Choice Based Credit System (CBCS)

B.Sc (Hons) Chemistry

University of Delhi

UNDERGRADUATE PROGRAMME

(Courses effective from Academic Year 20XX-XX)

SYLLABUS OF COURSES TO BE OFFERED: ***Core Courses, Elective Courses &Skill Enhancement Courses***

B.Sc. (Hons) Chemistry

Introduction

The Choice Based Credit System (CBCS) provides an opportunity to a student to choose courses from the syllabus comprising Core, Elective and Skill based courses. It offers a flexibility of programme structure while ensuring that the student gets a strong foundation in the subject and gains in depth knowledge. The learning outcome based curriculum framework will provide students with a clear purpose to focus their learning efforts and enable them to make a well judged choice regarding the course they wish to study. This will suit the present day needs of students in terms of securing their paths towards higher studies or employment.

Programme Duration and Design

The B.Sc. (Hons) Chemistry course is a six semester course spread over three academic years. The teaching – learning process involves theory and practical classes and will be student centered. Apart from the conventional chalk and talk method, power point presentations, audio – video tools, class discussions, simulations and virtual labs (wherever possible) will be used. Students will be encouraged to carry out short term projects and participate in industrial and institutional visits, seminars and workshops. Assessment will be based on continuous evaluation (class test, presentation, group discussion, quiz, assignment etc.) and end of semester examination. Each theory paper will be of 100 marks out of which 25% marks are reserved for internal assessment while a practical paper will be of 50 marks comprising 50% internal assessment.

Programme Structure

The programme includes Core Courses and Elective Courses. The Core Courses are all compulsory courses.There are three types of Elective Courses – Discipline Specific Elective (DSE), Generic Elective (GE), Skill Enhancement Courses (SEC). In addition there are two compulsory Ability Enhancement Courses (AEC). The Core, DSE and GE Courses are six credit courses; the SEC, AEC are four credit courses.

To acquire a B.Sc. (Hons) Chemistry degree, the student will study fourteen Core Courses, fourDiscipline Specific Elective Courses, four Generic Elective Courses, two Skill Enhancement Courses and two Ability Enhancement courses.

The student will study two Core Courses each, in Semesters I and II, three Core Courses each in Semesters III and IV and two Core Courses each in Semesters V and VI. The programme offers several Discipline-Specific Electives, of which the student will study two in each of the Semesters V and VI.

Different Generic Elective courses are offered to students of B.Sc. (Hons) Chemistry Programme by other Departments of the Collegeand the student will have the option to choose one GE course each in Semesters I, II, III, and IV. **At least two papers of Mathematics are compulsory for admission to**

M.Sc. Chemistry in University of Delhi, thus students are advised to opt for the same. The Department of Chemistry offers seven GE courses to students of other disciplines (refer to * on page 4).

Students will study one Skill Enhancement Course in Semesters III and IV. The two compulsory Ability Enhancement Courses are Environmental Sciences and English Communication and the student will study one each in Semesters I and II.

B.Sc. (H) CHEMISTRY PROGRAMME STRUCTURE AND COURSE DISTRIBUTION

Semester	Core Course (14)	Ability Enhancement Course (AEC) (2)	Skill Enhc. Course (SEC)(2)	Discipline Specific Elective (DSE) (4)	Generic Elective (GE) (4)
I	Inorganic Chemistry I:Atomic Structure & Chemical Bonding	Environmental Science / English Communication			GE-1
	Physical Chemistry I:States of Matter & Ionic Equilibrium				
II	Organic Chemistry I:Basics and Hydrocarbons	Environmental Science / English Communication			GE-2
	Physical Chemistry II:Chemical Thermodynamics and its Applications				
III	Inorganic Chemistry II:s- and p-Block Elements		SEC -1		GE-3
	Organic Chemistry II:Oxygen Containing Functional Groups				
	Physical Chemistry III:Phase Equilibria and Electrochemical Cells				
IV	Inorganic Chemistry III:Coordination Chemistry		SEC -2		GE-4
	Organic Chemistry III:Heterocyclic Chemistry				
	Physical Chemistry IV: Conductance & Chemical Kinetics				
V	Organic Chemistry IV: Biomolecules			DSE-1	
	Physical Chemistry V: Quantum Chemistry & Spectroscopy			DSE-2	
VI	Inorganic Chemistry IV: Organometallic Chemistry			DSE -3	

	Organic Chemistry V: Spectroscopy			DSE-4	

COURSES OFFERED UNDER B.Sc. (H) CHEMISTRY PROGRAMME (CBCS)

CORE COURSES –14 (six credits each) – Each course has 4 Periods/week for Theory, 4 Periods/week for Practical			
SEMESTER	**COURSE CODE**	**NAME OF THE COURSE**	**CREDITS T=Theory Credits P=Practical Credits**
I	CHEMISTRY – C I	Inorganic Chemistry I:Atomic Structure & Chemical Bonding	T=4 P=2
	CHEMISTRY – C II	Physical Chemistry I:States of Matter & Ionic Equilibrium	T=4 P=2
II	CHEMISTRY – C III	Organic Chemistry I:Basics and Hydrocarbons	T=4 P=2
	CHEMISTRY – C IV	Physical Chemistry II:Chemical Thermodynamics and its Applications	T=4 P=2
III	CHEMISTRY – C V	Inorganic Chemistry II:s- and p-Block Elements	T=4 P=2
	CHEMISTRY – C VI	Organic Chemistry II:Oxygen Containing Functional Groups	T=4 P=2
	CHEMISTRY – C VII	Physical Chemistry III:Phase Equilibria and Electrochemical Cells	T=4 P=2
IV	CHEMISTRY – C VIII	Inorganic Chemistry III:Coordination Chemistry	T=4 P=2
	CHEMISTRY – C IX	Organic Chemistry III:Heterocyclic Chemistry	T=4 P=2
	CHEMISTRY – C X	Physical Chemistry IV: Conductance & Chemical Kinetics	T=4 P=2
V	CHEMISTRY – C XI	Organic Chemistry IV: Biomolecules	T=4 P=2
	CHEMISTRY – C XII	Physical Chemistry V: Quantum Chemistry & Spectroscopy	T=4 P=2
VI	CHEMISTRY – C XIII	Inorganic Chemistry IV: Organometallic Chemistry	T=4 P=2
	CHEMISTRY – C XIV	Organic Chemistry V: Spectroscopy	T=4 P=2
			Credits: 14× 6 = 84
DISCIPLINE SPECIFIC ELECTIVE COURSES (DSE) – 4 (six credits each, refer to ** on page 5) Each course has 4 Periods/week for Theory, 4 Periods/week for Practical			
SEMESTER	**COURSE CODE**	**NAME OF THE COURSE**	**CREDITS T=Theory Credits P=Practical Credits**
V, VI		Novel Inorganic Solids	T=4 P=2
		Inorganic Materials of Industrial Importance	T=4 P=2
		Applications of Computers in Chemistry	T=4 P=2
		Analytical Methods in Chemistry	T=4 P=2
		Molecular Modelling & Drug Design	T=4 P=2
		Polymer Chemistry	T=4 P=2
		Research Methodology for Chemistry	T=5 P=1
		Green Chemistry	T=4 P=2
		Industrial Chemicals & Environment	T=4 P=2
		Instrumental Methods of Analysis	T=4 P=2
		Dissertation	6

			Credits: 4 × 6 = 24
GENERIC ELECTIVES COURSES (GE)– 4(six credits each) –Offered by other Departments **Each course has 4 Periods/week for Theory, 4 Periods/week for Practical**			
SEMESTER	**COURSE CODE**	**NAME OF THE COURSE**	**CREDITS** **T=Theory Credits** **P=Practical Credits**
I		GE 1	6
II		GE 2	6
III		GE 3	6
IV		GE 4	6
			Credits: 4 × 6 = 24
SKILL ENHANCEMENT ELECTIVE COURSES (SEC) – 2 (four credits each, refer to * on page 5)**			
SEMESTER	**COURSE CODE**	**NAME OF THE COURSE**	**CREDITS** **T=Theory Credits** **P=Practical Credits**
III-IV		IT Skills for Chemists	T=2 P=2
		Basic Analytical Chemistry	T=2 P=2
		Chemical Technology & Society	4
		Cheminformatics	T=2 P=2
		Business Skills for Chemists	4
		Intellectual Property Rights	4
		Analytical Clinical Biochemistry	T=2 P=2
		Green Methods in Chemistry	T=2 P=2
		Pharmaceutical Chemistry	T=2 P=2
		Chemistry of Cosmetics & Perfumes	T=2 P=2
		Pesticide Chemistry	T=2 P=2
		Fuel Chemistry	T=2 P=2
			Credits: 2 × 4 = 08
ABILITY ENHANCEMENT COURSES (AEC) – 2 (4 credits each)			
SEMESTER	**COURSE CODE**	**NAME OF THE COURSE**	**CREDITS** **T=Theory Credits** **P=Practical Credits**
I-II	AEC-I	Environmental Science	T = 4
	AEC-II	English Communication	T = 4
			Credits: 2 × 4 = 08
TOTAL CREDITS = 148			

***Generic Elective Papers (GE) for other Departments/Disciplines: (Credit: 06 each – 4T + 2P)**

1. Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons
2. Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I
3. Solutions, Phase Equilibrium, Conductance, Electrochemistry & Functional Group Organic Chemistry-II
4. Chemistry of s- and p-block elements, States of matter and Chemical Kinetics
5. Chemistry of d-block elements, Quantum Chemistry and Spectroscopy
6. Organometallics, Bioinorganic chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy

7. Molecules of life

****Discipline Specific Elective Courses: (Credit: 06 each) (4 courses to be selected)-DSE 1-4**

DSE 1: Any one of the following

1. Novel Inorganic Solids
2. Inorganic Materials of Industrial Importance

DSE 2: Choose any one of the following

1. Applications of Computers in Chemistry
2. Analytical Methods in Chemistry
3. Green Chemistry
4. Industrial Chemicals & Environment

DSE 3 and 4: Choose any one option each from Group A and Group B

Group A

1. Analytical Methods in Chemistry
2. Polymer Chemistry
3. Industrial Chemicals & Environment
4. Instrumental Methods of Analysis

Group B

1. Applications of Computers in Chemistry
2. Molecular Modelling & Drug Design
3. Research Methodology for Chemistry
4. Green Chemistry

All colleges will float more than one DSE course for DSE 2,3 and 4 to enable students to have a choice. Students may opt for a dissertation as a DSE course in Semester VI. It will be a six credit course. The number of students who will be allowed to opt for this will vary from college to college depending upon the infrastructural facilities and may vary each year. The college may announce the number of seats for project work well in advance and choose students for the same. It will involve experimental work under the supervision of a faculty member and will involve about eight hours of work a week. The project will be evaluated by internal and external examiners and the report should be sent to examiners in advance (prior to the day of examination).

*****Skill Enhancement Courses** - emphasis is given to **Hands on Exercises,** except for the following **papers which involve a Project**

- Chemical Technology & Society
- Business Skills for Chemists
- Intellectual Property Rights

Learning Outcome based approach to curriculum design

The Learning Outcomes-based Curriculum Framework (LOCF) for the B.Sc. (Hons) degree in Chemistry provides a broad structural framework that can accommodate the current curricular needs as well as gives sufficient flexibility to include changes in content that assume importance as the frontiers of science grow. The inherent flexibility in framework allows design of course basket in tune with individual preferences. The basic uniformity in core course design ensures smooth movement across universities in the country. The B.Sc. (Honours) Chemistry programme covers a wide range of basic and applied courses as well as courses of interdisciplinary nature. While the core courses aim to build a strong conceptual chemical knowledge base in the student, the contents of electives and skill enhancement courses help them explore their fitness and suitability to pursue studies in these areas.

Attributes of a graduate in chemistry

Though a student pursuing an undergraduate degree in a science discipline is inherently curiosity driven, has the ability to observe and integrate rationally, a student graduating with an honours degree in chemistry is distinguished by the following additional attributes:

- **Sound knowledge of the discipline**: Has acquired in-depth knowledge of the various concepts and theoretical principles and is aware of their manifestations. An understanding of the centrality of chemistry is usually evident from familiarity with interfacial disciplines.
- **Laboratory skills and techniques**: A graduate in chemistry is expected to be thoroughly conversant with all basic analytical, qualitative and quantitative laboratory techniques and demonstrate meticulousness in operations.
- **Digital literacy**: Increasing use of instruments having interface with computers and use of computers in laboratory work creates this attribute. A student with degree in chemistry is able to employ knowledge and skill in computers in a variety of situations- data analysis, computing as well as information retrieval and library use.
- **Team player/ interpersonal skills:** Capable of contributing meaningfully to team ethos and goals. Teams may comprise of peers in classroom, laboratory or any other team of members from diverse fields.
- **Critical thinking:** An integral part of chemistry curriculum is problem solving. Problems of numerical, synthetic and analytical nature are best approached with critical thinking. Critical thinking as an attribute enables a student to analyze a problem, assess it, reconstruct it and solve it.
- **Effective communicator:** Effective communication is a much desirable attribute across courses. However, a chemistry honours student is expected to assimilate technical information about chemistry from various sources and convey to intended audience, both orally and in writing in an intelligible manner.
- **Awareness of ethical issues:** Is aware of what constitutes unethical behaviour-- plagiarism, fabrication and misrepresentation or manipulation of data.

- **Safety and environmental concerns:** Is aware of the importance of working with safety consciousness in laboratory. Actively seeks information about health and environmental safety of chemicals that are used in the laboratories and follows protocols for their safe disposal.
- **Research oriented:** Is inquisitive about processes and phenomena happening during experiments in laboratories and seeks answers through the research path.

Qualification descriptors

The qualification description for B.Sc. (Hons) programme in Chemistry includes

- Demonstration of a comprehensive knowledge base in concepts, principles and theories related to chemistry that spans the traditional sub-disciplines (inorganic chemistry, organic chemistry, physical chemistry, analytical chemistry and biochemistry) as well as advanced and emerging topics.
- Demonstration of an ability to apply underlying concepts and principles outside the context in which they were first studied and in interdisciplinary scenarios.
- Acquisition of competence in the use of routine materials, techniques and practices of chemistry.
- Exhibition of skills required for the conduct of documented laboratory procedures as well as well-developed skills for the gathering, evaluation, analysis and presentation of information, ideas, concepts and quantitative and/or qualitative data.
- Acquisition of skills in the operation of standard chemical instrumentation.
- Demonstration of skills in the use of safety data sheets, safe-handling of chemical materials, considering their physical and chemical properties including any specific hazards associated with their use.
- Development of literature searching and information management skills.
- Acquisition of the ability for responsible treatment of data, proper citation of others' work, and the standards related to plagiarism.
- Development of awareness of the role of chemistry in contemporary societal and global issues, including areas such as sustainability and green chemistry.
- Development of the appreciation of the uses of chemistry in daily life.
- Development of competence in intellectual, practical and transferable skills (Communication skills, IT skills, Interpersonal skills) necessary for a professional chemist.

Programme learning outcomes

The B.Sc.(Hons) programme in Chemistry is designed to develop in students in depth knowledge of the core concepts and principles that are central to the understanding of this core science discipline. 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.

- **Knowledge: Width and depth:** Students acquire theoretical knowledge and understanding of the fundamental concepts, principles and processes in main branches of chemistry, namely, organic chemistry, inorganic chemistry, physical chemistry, analytical chemistry and biochemistry. Depth in understanding is the outcome of transactional effectiveness and treatment of specialized course contents. Width results from the choice of electives that students are offered.
- **Laboratory Skills: Quantitative, analytical and instrument based:** A much valued learning outcome of this programme is the laboratory skills that students develop during the course. Quantitative techniques gained through hands on methods opens choice of joining the industrial laboratory work force early on. 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 cross branches to join analytical, pharmaceutical, material testing and biochemical labs besides standard chemical laboratories.
- **Communication:** Communication is a highly desirable attribute to possess. Opportunities to enhance students' 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 chemistry honours programme 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 chemistry honours 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.

Teaching – Learning Process

B.Sc. (Hons) Chemistry programme is a three-year degree programme designed to provide students with a sound theoretical background and practical training in all aspects of chemistry and helps them develop an appreciation of the importance of chemistry in different contexts. The programme includes foundational as well as in-depth courses that span the traditional sub-disciplines of chemistry. Along with the above Core Courses there are Discipline Specific Elective Courses, Generic Elective Courses and Ability Enhancement Courses which address the need of the hour.

These courses are delivered through classroom, laboratory work, projects, case studies and field work in a challenging, engaging, and inclusive manner that accommodates a variety of learning styles and tools (PowerPoint presentations, audio visual resources, e-resources, seminars, workshops, models, softwares).

The laboratory training complements the theoretical principles learned in the classroom and includes synthesis of molecules, measurement of chemical properties and phenomenon, hands-on experience with modern instruments, computational data analysis, modelling and laboratory safety procedures.

Different pedagogies such as problem-based learning, peer-led instruction, and technology-aided instruction (blended learning) are adopted wherever suitable. These promote independent thinking, critical thinking and reasoning and a perspective of chemistry as a scientific process of discovery. Students are encouraged to work together in groups which leads to development of interpersonal skills like communication and team work.

The student will participate in industrial visits that will lay strong foundation for a successful career as a professional chemist by providing him useful information related to the practical aspects of the course and giving an insight to future areas of employment.

Assessment Methods

Assessment methods have two major objectives:

- The primary one is to assess the learning outcomes of the course in tune with the broad outcomes of strengthening core theoretical knowledge base and practical laboratory skills. This is assessed by comprehensive summative end-semester examinations conducted for both theory and laboratory courses. Also In-courseassessmentsare given in every course in order to assess the students mastery of various learning outcomes. These assessments include individual assignments, group assignments, laboratory notebooks, written reports, quizzes, class tests and periodical tests.
- Another objective is to improve the students' learning and teachers' teaching. Results of assessments and their critical analysis are used to improve the process further by focusing on the areas that need conceptual strengthening, laboratory exposure or design of new experiments.

CORE COURSE (HONOURS IN CHEMISTRY)

INORGANIC CHEMISTRY

SEMESTER 1

CHEMISTRY - C I: INORGANIC CHEMISTRY - I
Atomic Structure & Chemical Bonding
Total Credits: 06 (Credits: Theory-04, Practicals-02)
(Total Lectures: Theory- 60, Practicals-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.

Learning Outcomes:

By the end of the course, the students will be-

1. 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.
2. Able to draw the plausible structures and geometries of molecules using Radius Ratio Rules, VSEPR theory and MO diagrams (homo- & hetero-nuclear diatomic molecules).
3. Able to understand the concept of lattice energy using Born-Landé and Kapustinskii expression.
4. Able to rationalize the conductivity of metals, semiconductors and insulators based on the Band theory.
5. Able to understand the importance and application of chemical bonds, inter-molecular and intra-molecular weak chemical forces and their effect on melting points, boiling points, solubility and energetics of dissolution.

Unit 1:

Atomic Structure: Recapitulation of Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance.

Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, and *d o*rbitals.

Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau principle and its limitations.

(**Lectures : 14)**

Unit 2:

Periodicity of Elements: Brief discussion of the following properties of the elements, with reference to *s* & *p*-block and the trends shown:

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.
(b) Atomic and ionic radii
(c) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization enthalpy and trends in groups and periods.
(d) Electron gain enthalpy and trends in groups and periods.
(e) Electronegativity, Pauling's/ Allred Rochow's scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity.

(**Lectures : 16)**

Unit 3:

Chemical Bonding

Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy.

(Lectures : 7)

Unit 4:

Covalent bond*:* Lewis structure, Valence Bond theory (*Heitler-London* approach). Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2, O_2, C_2, B_2, F_2, CO, NO, and their ions; HCl (idea of s-p mixing and orbital interaction to be given).

(**Lectures : 8)**

Unit 5:

VSEPR Theory :Valence shell electron pair repulsion theory (VSEPR), shapes of the following simple molecules and ions containing lone pairs and bond pairs of electrons: H_2O, NH_3, PCl_3, PCl_5, SF_6, ClF_3, I_3^-, BrF^{2+}, PCl_6^-, ICl_4^-, and SO_4^{2-}.
Multiple bonding (s and π bond approach) and bond lengths.
Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.
Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(**Lectures : 10)**

Unit 6:

Metallic Bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.

Weak Chemical Forces: Van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interaction, Hydrogen bonding (theories of hydrogen bonding, valence bond treatment).
Effects of weak chemical forces, melting and boiling points, solubility, energetics of dissolution process.

(**Lectures: 05)**

Practical:

(Credits: 02, Lectures: 60)

1. Titrimetric Analysis : (i) Calibration and use of apparatus (ii) Preparation of solutions of titrants of different Molarity/Normality.

2. Acid-Base Titrations : Principles of acid-base titrations to be discussed.

(i) Estimation of sodium carbonate using standardized HCl.

(ii) Estimation of carbonate and hydroxide present together in a mixture.

(iii) Estimation of carbonate and bicarbonate present together in a mixture.

(iv) Estimation of free alkali present in different soaps/detergents

3. Oxidation-Reduction Titrimetry : Principles of oxidation-reduction titrations (electrode potentials) to be discussed.

(i) Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$ solution

(ii) Estimation of oxalic acid and sodium oxalate in a given mixture.

(iii) Estimation of Fe(II) with $K_2Cr_2O_7$ using internal indicator (diphenylamine, N-phenylanthranilic acid) and discussion of external indicator.

References

Theory:

Concise Inorganic Chemistry, Lee, J.D., Fifth Edn., Wiley India.India.

I*norganic Chemistry- Principles of Structure and Reactivity*, Huheey, J.E., Keiter, E.A., Keiter, R. L., Medhi, O.K., Pearson Education 2009.

Concepts and Models of Inorganic Chemistry,Douglas, B.E., McDaniel, D.H., Alexander, J.J., 3rd Edn., John Wiley & Sons, Inc. 1993.

Shriver and Atkins' Inorganic Chemistry,

P.W. Atkins, T.L. Overton, J.P. Rourke, M.T. Weller, and F.A. Armstrong, 5th Edn,©2010, W. H. Freeman and Company, 41 Madison Avenue, New York, NY 10010 www.whfreeman.com.

Inorganic Chemistry, Miessler, Gary L., Fischer Paul J., Tarr, Donald A., Fifth edition, Pearson, 2014.

Practicals:

***Vogel's Textbook of Quantitative Chemical Analysis*, Jeffery, G.H., Bassett, J., Mendham, J., Denney, R.C., 5th Edn.,** Longman Scientific & Technical, England, *(John Wiley and Sons Inc, 605 Third Avenue, New York NY 10158).*

Additional Resources:
Inorganic Chemistry, Wulfsberg, Gary, Viva Books Private Limited, India, 2002. .

Teaching Learning Process

- Conventional chalk and board teaching,
- Class interactions and discussions
- Power point presentation on important topics.

Assessment Methods

- Presentations by Individual Student/ Group of Three Students
- Class Tests at Periodic Intervals.
- Written assignment(s)
- End semester University Theory and Practical Examination

Keywords

Atomic Structure, Wave function, Quantum Numbers, Electronegativity, Ionic Bonding, Dipole Moment, VESPER Theory, Covalent Bonding, Multiple Bonding, Bonding Molecular Orbitals, Bonding MO, Antibonding MO, Homonuclear, Hetronuclear, Metallic Bonding, Weak Chemical Forces

CHEMISTRY - C II: PHYSICAL CHEMISTRY - I
States of Matter & Ionic Equillibrium

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

Objectives:

1. Understand states of matter and interchange of states, intermolecular interactions.
2. Understand state of equilibrium, concept of pH, buffers, acids and bases indicators.

Learning Outcomes:

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

- Explain the difference between solid, liquid and gases in terms of intermolecular interactions.
- Apply the concepts of gas equations, pH and electrolytes while studying other chemistry courses.
- Explain buffers and use them in different experiments.

Unit 1:

Gaseous state: Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of σ from η; variation of viscosity with temperature and pressure. Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities. Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, Z, and its variation with pressure and temperature for different gases. Causes of deviation from ideal behaviour. Equation of states for real gases; van der Waals equation of state, its derivation and application in explaining real gas behaviour, Virial coefficients, calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states.

(Lectures: 22)

Unit 2:

Liquid state: Qualitative treatment of the structure of the liquid state; physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various

solutes on surface tension and viscosity. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases.

(Lectures: 06)

Unit 3:

Solid state: Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl.

Unit 4:

Ionic equilibria: Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono and diprotic acids. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts.

Buffer solutions; derivation of Henderson equation and its applications. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

(Lectures: 20)

Practical:

(Credits: 02,Lectures: 60)

1. *Surface tension measurements using stalagmometer.*

a. Determine the surface tension of aqueous solutions by (i) drop number (ii) drop weight method.

b. Study the variation of surface tension with different concentration of detergent solutions. Determine CMC.

2. *Viscosity measurement using Ostwald's viscometer.*

a. Determination of co-efficient of viscosity of an unknown aqueous solution.

b. Study the variation of co-efficient of viscosity with different concentration of Poly Vinyl Alcohol (PVA) and determine molar of PVA.

b. Study the variation of viscosity with different concentration of sugar solutions.

3. *Solid State:*

a. Indexing of a given powder diffraction pattern of a cubic crystalline system.

4. *pH metry:*

a. Study the effect of addition of HCl/NaOH on pH to the solutions of acetic acid, sodium acetate and their mixtures.

b. Preparation of buffer solutions of different pH values (i) Sodium acetate-acetic acid (ii) Ammonium chloride-ammonium hydroxide

c. pH metric titration of (i) strong acid with strong base, (ii) weak acid with strong base and determination of dissociation constant of a weak acid.

Any other experiment carried out in the class.

References:

Theory

- Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry Ed., Oxford University Press 10th Ed (2014).
- Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).
- Thomas Engel & Philip Reid Physical Chemistry Pearson Education 3rd Ed(2013)
- Barrow, G. M. Physical Chemistry
- Kapoor, K.L., Physical Chemistry 6th Ed Vol 1

Practical

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Additional Resources:

- Walter J. Moore Physical Chemistry 5th Ed (1972)
- Samuel Glasstone Textbook of Physical Chemistry

Teaching Learning Process:

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

- Explain the concepts using conventional methods of teaching, models and simulations
- Guide the students in solving relevant problems

- Application of the concepts to explain real life phenomenon
- Guiding the students to interpret the observations and results in the practicals
- Correlating the experiments performed in the practicals with the concepts learned in theory

Assessment Methods:

- Assignments
- Oral and written tests
- Presentations
- Semester end examination

Keywords:

States of matter, ideal gas, real gas, van der waals equation of state, mean free path, Maxwell distribution, critical constants, viscosity, surface tension, liquids, crystal, symmetry, lattice, crystal system, Miller indices, X-ray diffraction, Bragg's law, crystal structure, NaCl, CsCl, KCl, ionic equilibria, weak and strong electrolytes, weak acid, weak base, hydrolysis, solubility product, pH, titrations, indicator

---

SEMESTER II

CHEMISTRY - CIII: ORGANIC CHEMISTRY I
Basics and Hydrocarbons

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

Objectives:

The core course Organic Chemistry I isdesigned in a manner that it forms a cardinal part of the learning of organic chemistry for the subsequent semesters. The course is 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 functional groups- 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 Objectives:

On the completion of the course, the student will be able to do the following:

1. Understand and explain the differential behavior of organic compounds based on fundamental concepts learnt.
2. Formulate the mechanism of organic reactions by recalling and correlating the fundamental properties of the reactants involved.
3. Learn and identify many organic reaction mechanisms including Free Radical Substitution,Electrophilic Addition and Electrophilic Aromatic Substitution.
4. Correlate and describe the stereochemical properties of organic compounds and reactions.

Unit 1:

Recapitulation of Basics of Organic Chemistry

Hybridisation: Shapes of molecules

Electronic Displacements and their applications: Inductive, Electromeric, Resonance and Mesomeric effects and Hyperconjugation.

Concept of dipole moment, Acidity and Basicity and related pKa values.
Homolytic and heterolytic fissions with suitable examples, types, shape and relative stability of Carbocations, Carbanions, Free radicals and Carbenes.
Weaker forces like van der Waal's forces and Hydrogen bonding
Electrophiles and Nucleophiles and introduction to types of organic reactions: Addition, Elimination and Substitution reactions.

(6 Lectures)

Unit 2:

Stereochemistry

Stereoisomerism: Optical Activity and Optical Isomerism, Asymmetry, Chirality, Enantiomers, Diastereomers. specific rotation; Configuration and Projection Formulae: Newmann, Sawhorse, Fischer and their interconversion. Chirality in molecules with one and two stereocentres and with no stereocentre (Allenes, biphenyls); meso configuration. Racemic modification and their resolution. Relative and absolute configuration: D/L and R/S designations. Geometrical isomerism: cis-trans, syn-anti and E/Z notations with CIP rules.

(18 Lectures)

Unit 3:

Carbon-Carbon sigma bonds (Alkanes and Cycloalkanes)

General methods of preparation- Wurtz and Wurtz Fittig reaction, Corey House synthesis, physical and chemical properties of alkanes, Isomerism and its effect on properties of molecule, Free radical substitutions; Halogenation, concept of relative reactivity v/s selectivity. Conformational analysis of alkanes (Conformations, relative stability and energy diagrams of Ethane, Propane and butane).General molecular formulae of cycloalkanes and relative stability, Baeyer strain theory, Cyclohexane conformations with energy diagram, Axial and equatorial positions. Conformations of

monosubstituted alkanes.

(16 Lectures)

Unit 4:

Carbon-Carbon pi Bonds (Alkenes and Alkynes)

Structure and isomerism .General methods of preparation, physical and chemical properties. Mechanism, of E1, E2, E1cb reactions, Saytzeff and Hoffmann eliminations, Electrophilic Additions , mechanism with suitable examples, (Markownikoff/Antimarkownikoff addition), *syn* and *anti* addition; addition of H_2, X_2, methylene, oxymercuration-demercuration, hydroboration-oxidation, ozonolysis, hydroxylation, Diels Alder reaction, 1,2-and 1,4-addition reactions in conjugated dienes.

Mechanism of allylic and benzylic bromination in propene, 1-butene, toluene,ethyl benzene.
Reactions of alkynes; acidity, electrophilic and nucleophilic additions, hydration to form carbonyl compounds, Alkylation of terminal alkynes.

(8 Lectures)

Unit 5:

Aromatic Hydrocarbons

Concept of Aromaticity: Huckel's rule, aromatic character of arenes, cyclic carbocations/ carbanions and heterocyclic compounds with suitable examples. Electrophilic aromatic substitution: halogenation, nitration, sulphonation, Friedel Crafts alkylation/ acylation with their mechanism. Directing effects of groups in electrophilic substitution.

(12 Lectures)

Practical:

Credit: 2, Lectures: 60

1. Organic Preparation (any one of the following):
    a. Bromination of acetanilide/aniline/phenol
    b. Nitration of nitrobenzene/toluene
2. Calibration of a thermometer
3. Purification of organic compounds by crystallization using the following solvents:
    a. .Water
    b. Alcohol
    c. Alcohol-Water
4. Determination of the melting points of prepared organic compounds (Kjeldahl method and electrically heated melting point apparatus)
5. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds
6. Determination of boiling point of liquid compounds. (boiling point lower than and more than 100 °C by distillation and capillary method)
7. Chromatography

(a) Separation of a mixture of two amino acids by ascending and radial paper chromatography

(b) Separation of a mixture of two sugars by ascending paper chromatography
(c) Separation of a mixture of o-and p-nitrophenol or o-and p-aminophenol by thin layer chromatography (TLC)

8. Detection of extra elements

References:

Theory:

- Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds; Wiley: London, 1994.
- Kalsi, P. S. Stereochemistry Conformation and Mechanism; New Age International, 2005.
- Practical
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)

Practical:

- Ahluwalia, V.K. &Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- Ahluwalia, V.K. & Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

Additional Resources:

- Solomons, T. W. G.; Fryhle, C. B. & Snyder, S. A. Organic Chemistry, 12th Edition, Wiley.
- Bruice, P. Y. Organic Chemistry, Eighth Edition, Pearson.
- Clayden, J.; Greeves, N. & Warren, S. Organic Chemistry, Oxford.
- Nasipuri, D. Stereochemistry of Organic Compounds: Principles and Applications, Third Edition, New Age International.
- Gunstone, F. D. Guidebook to Stereochemistry, Prentice Hall Press, 1975.

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:

- Continuous Evaluation: Monitoring the progress of student's learning
- Class Tests, Worksheets and Quizzes
- Presentations, Projects and Assignments and Group Discussions: Enhances critical thinking skills and personality
- Semester-end Examination: critical indicator of student's learning and teaching methods adopted by teachers throughout the semester.

Keywords:

Stereochemistry, Alkanes, Alkenes, Cycloalkanes, Alkynes, Aromatic Hydrocarbons

---

CHEMISTRY - C IV: PHYSICAL CHEMISTRY - II
Chemical Thermodynamics and its Applications

Total Credits: 06 (Credits: Theory-04, Practicals-02)
(Total Lecture: Theory- 60, Practicals-60)

Objectives:

1.The aim of this course is to make students understand the concepts of energy, heat, work, enthalpy, entropy, free energies and the relation between them.

2. To apply these processes, extend the thermodynamic properties to the system of variable compositions, equilibrium and colligative properties.

Learning Outcomes:

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

- Understand the three laws of thermodynamics, concept of State and Path functions, extensive and intensive properties.
- Derive the expressions of ΔU, ΔH, ΔS, ΔG, ΔA for ideal gases under different conditions.
- Explain the concept of partial molar properties.
- Derive the expression of equilibrium constants.
- Explain the thermodynamic basis of colligative properties.

Unit 1:

Chemical Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems.

Mathematical Manipulation - Exact and inexact differential, Partial derivatives, Eular's reciprocity rule, cyclic rule.

(Lectures: 6)

Unit 2:

First law: Concept of heat, Q, work, W, internal energy, U, and statement of first law; enthalpy, H, relation between heat capacities), calculations of Q, W, ΔU and ΔH for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions.

Thermochemistry: Heats of reactions: standard states; enthalpy of neutralisation, enthalpy of hydration, enthalpy of formation and enthalpy of combustion and its applications, bond dissociation energy and bond enthalpy; effect of temperature (Kirchhoff's equations) on enthalpy of reactions.

(Lectures: 14)

Unit 3:

Second Law: Concept of entropy; statement of the second law of thermodynamics, Carnot cycle . Calculation of entropy change for reversible and irreversible processes (for ideal gases). Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity (for ideal gases). Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

(**Lectures: 16)**

Unit 4:

Third Law: Statement of third law, unattainability of absolute zero, calculation of absolute entropy of molecules, concept of residual entropy.

(**Lectures: 04**)

Unit 5:

Systems of Variable Composition: Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs Duhem equation, chemical potential of ideal mixtures. Change in thermodynamic functions on mixing of ideal gases.

Chemical Equilibrium: Criteria of thermodynamic equilibrium, degree of advancement of reaction.Chemical equilibria in ideal gases. Thermodynamic derivation of relation between Gibbs free energy of a reaction and reaction quotient. Equilibrium constants and their dependence on temperature, pressure and concentration . LeChatelier Principle (Quantitative treatment).Free energy of mixing and spontaneity. Equilibrium between ideal gases and a pure condensed phase.

(Lectures :10)

Unit 6:

Solutions and Colligative Properties: Dilute solutions; lowering of vapour pressure, Raoult's law. Thermodynamic basis of the colligative properties - lowering of vapour pressure, elevation of Boiling Point, Depression of Freezing point and Osmotic pressure and derivation of expressions for these using chemical potential. Application of colligative properties in calculating molar masses of normal, dissociated and associated solutes in solutions.

(Lectures:10)

Practical:

(Credits: 2, Lectures: 60)

Thermochemistry:
(a) Determination of heat capacity of a calorimeter for different volumes using (i) change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of neutralization), and (ii) heat gained equal to heat lost by cold water and hot water respectively
(b) Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
(c) Determination of the enthalpy of ionization of ethanoic acid.
(d) Determination of integral enthalpy (endothermic and exothermic) solution of salts.
(e) Determination of basicity of a diprotic acid by the thermochemical method for different additions of a base
(f) Determination of enthalpy of hydration of salt.

References:

Theory:

- Peter, A. & Paula, J. de. Physical Chemistry 9th Ed., Oxford University Press (2011).
- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- McQuarrie, D. A. & Simon, J. D. Molecular Thermodynamics Viva Books Pvt. Ltd.: NewDelhi (2004).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly asked Questions in Thermodynamics. CRC Press: NY (2011).
- Levine, I .N. Physical Chemistry 6th Ed., Tata Mc Graw Hill (2010).
- Metz, C.R. 2000 solved problems in chemistry, Schaum Series (2006) Practical

Practicals:

- Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Athawale, V. D. &Mathur, P. Experimental Physical Chemistry New Age International: New Delhi (2001).
- Atkins, P, Paula J.D., Elements of Physical Chemistry, Oxford University Press, (2013)
- Glasstone, S. Textbook of Physical Chemistry, Mcmillan,Canada (1948)
- Kapoor, K.L. A Textbook of Physical Chemistry, Vol II, McGraw Hill Education (India) (2011)
- Kapoor, K.L. A Textbook of Physical Chemistry, Vol III, McGraw Hill Education (India) (2012)
- Glasstone, S. Thermodynamics for Chemists, Affileated East West Press Pvt. Ltd. (1947)

Teaching Learning Process:

1. Interactive teaching methods to be used. Each topic should be presented by the teacher, followed by discussion after giving the students sufficient time for self study. Multimedia may be used if it enhances the quality of presentation e,g., where 3 D visualization is required.

2. Conceptual and numerical problems should be discussed in the class and active participation of students should be encouraged.

3. Group work may be introduced. The class is divided into groups of 3-4 students. Each group is given a problem which they discuss and solve and present the solution to the class. This may be followed by the whole class participating in the discussion.

4. In lab work the students should be told beforehand about the experiment to be performed. They should be expected to come prepared with the conceptual and procedural part of the experiment. This can then be discussed before start of the practical. Special emphasis should be on sources of error and results of all students/groups may be compared in the end. Sources of error and how to avoid them with appropriate precautions should also be discussed.

Assessment Methods:

Students are expected to explain things rather than proving through derivations.

Frequent short quiz to test conceptual understanding,Open book assignments in class, Group presentation. In lab work assessment is based on a. conceptual understanding b. Presentation of data c. Internal consistency d. Result (taking into consideration the unavoidable errors)

Evaluation for practicals - a) Internal Assessment should be 25%

b) Practical Component 50%,

c) Viva 25%

Keywords:

Thermodynamics, State Functions, Path Functions, Energy, Heat, Work, Enthalpy, Entropy, Gibb's Free energy, Equilibrium, Spontaneity, Irreversible, Work Function, Chemical Potential, Partial Molar Quantities, Le Chatelier Principle, Colligative Properties

SEMESTER III

CHEMISTRY - CV: INORGANIC CHEMISTRY - II
s- and p-Block Elements

Total Credits: 06 **(Credits: Theory-04, Practicals-02)**
(Total Lecture: Theory- 60, Practicals-60)

Objectives:

The course reviews the general principals of Metallurgy and s-, p-block elements. It reviews the terms minerals, ores, concentration, benefaction, calcination, roasting, refining, etc and explains the principles of oxidation and reduction as applied to the extraction procedures. Methods of purification of metals,suchas electrolytic,oxidative refining, Van-Arkel De boer process and Monds process are discussed and applications of thermodynamic concepts like that of Gibbs energy and entropy to the extraction of metals are reviewed. It further discussed the patterns and trends exhibited by s and p block elements and their compounds with emphasis on synthesis, structure, bonding and uses.

Learning Outcomes:

By the end of the course, the students will be-

1) Able to learn the fundamental principles of metallurgy and will be in a position to ascertain the method of extraction of a particular metal and also understands the importance of recovery of byproducts during extraction.

2) Able to understandthe basic and practical applications in various fields of metals and alloy behavior and their manufacturing processes. They are further able to understand why alloys are preferred over metal alone

3) Able to apply the thermodynamic concepts like that of Gibbs energy and entropy to the principles of extraction of metals, such as Al, Cu, Zn and Fe;and also understand why specific reducing agents are used for reduction purposes.

4) Able to understand the periodicity in atomic and ionic radii, electronegativity, ionization energy, electron affinity of elements of the periodic table.

5) Able to understand Oxidation states with reference to elements in unusual and rare oxidation states like carbides and nitrides.

6) Able to understand vital role of Sodium, Potassium, Calcium and magnesium in biological systems and the use of caesium in devising photoelectric cells.

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 and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy with reference to cyanide process for silver and gold. Methods of purification of metals: Electrolytic process, van Arkel-de Boer process, Zone refining.

(6 Lectures)

Unit 2:

Chemistry of s-Block Elements:

- General characteristics: melting point, flame colour, reducing nature, diagonal relationships and anomalous behavior of first member of each group.
- Reactions of alkali and alkaline earth metals with oxygen, hydrogen, nitrogen and water.
- Common features such as ease of formation, thermal stability and solubility of the following alkali and alkaline earth metal compounds: hydrides, oxides, peroxides, superoxides, carbonates, nitrates, sulphates.
- Complex formation tendency of s-block elements; structure of the following complexes: crown ethers and cryptates of Group I; basic beryllium acetate, beryllium nitrate, EDTA complexes of calcium and magnesium.
- Solutions of alkali metals in liquid ammonia and their properties.

(22 Lectures)

Unit 3:

Chemistry of p Block Elements: Electronic configuration, atomic and ionic size, metallic/non-metallic character, melting point, ionization enthalpy, electron gain enthalpy, electronegativity, Catenation, Allotropy of C, P, S; inert pair effect, diagonal relationship between B and Si and anomalous behaviour of first member of each group.

(6 lectures)

Unit 4:

Structure, bonding and properties: acidic/basic nature, stability, ionic/covalent nature,oxidation/reduction, hydrolysis, action of heat of the following:

- Hydrides: hydrides of Group 13 (only diborane), Group 14, Group 15 (EH_3 where E = N, P, As, Sb, Bi), Group 16 and Group 17.
- Oxides: oxides of phosphorus, sulphur and chlorine
- Oxoacids: oxoacids of phosphorus and chlorine; peroxoacids of sulphur
- Halides: halides of silicon and phosphorus

(15Lectures)

Unit 5:

Preparation, properties, structure and uses of the following compounds:

- Borazine
- Silicates, silicones,
- Phosphonitrilic halides {(PNCl2)n where n = 3 and 4}
- Interhalogen and pseudohalogen compounds
- Clathrate compounds of noble gases, xenon fluorides (MO treatment of XeF2).

(11 Lectures)

Practical:

(Credits: 02, Lectures: 60)

(A) Iodo / Iodimetric Titrations

(i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodometrically).
(ii) Estimation of antimony in tartar-emetic iodimetrically
(iii) Estimation of Iodine Content in iodized salt

(B) Complexometric titrations using disodium salt of EDTA

(i) Estimation of Mg^{2+},Zn^{2+}
(ii) Estimation of Ca^{2+} by substitution method
(iii) Estimation of Calcium content in milk.

(C)Principles involved in chromatographic separations may be included:

Paper cinematographic separation of following metal ions:

a) Ni (II) and Co (II)
b) Cu(II) and Cd(II)

(C) Inorganic preparations

(i) Cuprous Chloride, Cu_2Cl_2
(ii) Aluminium potassium sulphate $KAl(SO_4)_2$.$12H_2O$ (Potash alum) or Chrome alum.

References:

- Douglas, B.E; Mc Daniel, D.H. & Alexander J. J. Concepts
- Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 3 rd Ed.(adapted), Pearson, 2009
- Shriver, D.F., Atkins P.W and Langford, C.H., Inorganic Chemistry 2 nd Ed., Oxford University Press, 1994
- Huheey, J.E., Keiter, E.A., Keiter, R. L., Medhi, O.K. Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education 2006.
- Lee, J.D., Concise Inorganic Chemistry, Pearson Education, 2010.

Assessment Methods:

(1) Test / Examination

(2) Assignment
(3) projects based on the real world application of important elements and their compounds
(4) quiz

Keywords: s-block elements, p-block elements, metallurgy, Ellingham Diagram, Zone Refining, Borazine, Silicates, Interhalogen, Pseudohalogen compounds.

CHEMISTRY - CVI: ORGANIC CHEMISTRY - II
Oxygen Containing Functional Groups
Total Credits: 06 (Credits: Theory-04, Practicals-02)
(Total Lectures: Theory- 60, Practicals-60)

Objectives:

The core course Organic Chemistry II is designed in a manner that gives a better understanding of the organic functional groups, which include halogenated hydrocarbons and oxygen containing functional groups and their reactivity patterns. The detailed reactions mechanistic pathways for each functional group will be discussed to unravel the spectrum of organic chemistry and the extent of organic transformations.

Learning Outcomes:

On the completion of the course, the student will be able to do the following:

1. Understand preparation, properties and reactions of haloalkanes, haloarenes and oxygen containing functional groups.
2. Use the synthetic chemistry learnt in this course to do functional group transformations.
3. To propose plausible mechanisms for any relevant reaction

Unit 1:

Chemistry of Halogenated Hydrocarbons:

Alkyl halides: Methods of preparation and properties, nucleophilic substitution reactions – S_N1, S_N2 and S_NI mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.

Aryl halides: Preparation (including preparation from diazonium salts) and properties, nucleophilic aromatic substitution; S_NAr, Benzyne mechanism.
Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Organometallic compounds of Mg (Grignard reagent) – Use in synthesis of organic compounds.

(16 Lectures)

Unit 2:

Alcohol, Phenol, Ether and Epoxides

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, BouvaeltBlancReduction; Oxidation of diols by periodic acid and lead tetraacetate, PinacolPinacolone rearrangement;

Phenols: Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer–Tiemann and Kolbe's–Schmidt Reactions, Fries and Claisen rearrangements with mechanism;

Ethers and Epoxides: Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and $LiAlH_4$

(16 Lectures)

Unit 3:

Carbonyl Compounds

Structure, reactivity, preparation and properties;

Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism.

Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisan-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and BenzilBenzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α - substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner,LiAlH4, $NaBH_4$, MPV, PDC)
Addition reactions of α, β- unsaturated carbonyl compounds: Michael addition.

Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

(16 Lectures)

Unit 4:

Carboxylic Acids and their Derivatives

General methods of preparation, physical properties and reactions of monocarboxylic acids, effect of substituents on acidic strength. Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids.
Preparation and reactions of acid chlorides, anhydrides, esters and amides;

Comparative study of nucleophilic sustitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann- bromamide degradation and Curtius rearrangement.

(12 Lectures)

Practical:
(Credits: 2, Lectures: 60)

1.Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group
2. Organic Preparations

i. Acetylation of one of the following compounds: amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and phenols (β -naphthol, vanillin, salicylic acid) by any one method:

a. Using conventional method.
b. Using green approach

ii. Benzolyation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and one of the following phenols (β -naphthol, resorcinol, p- cresol) by Schotten-Baumann reaction.

iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).

iv. Selective reduction of meta dinitrobenzene to m-nitroaniline.

v. Hydrolysis of amides and esters.

vi. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.

vii. S-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).

viii. Aldol condensation using either conventional or green method.The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization and melting point.

References:

Theory:

- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc
- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)

Practical:

- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
- Ahluwalia, V.K. &Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- Ahluwalia, V.K. & Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

Teaching Learning Process:

Following an outcome-based methodology to develop the requisite knowledge, skills, attitudes and habits of students, the following variables will be employed for an effective teaching learning process

Lectures:

- Assignments / Tests for the topics covered
- Discussion of previous years' examination question papers on completion of a particular topic.
- Seminars/ Group discussion
- Power point presentations
- Audio Visual aids
- Video lectures
- Hand- outs for specific topics
- Downloaded videos for animated experimental demonstration
- 3-D models

Practical:

- Classroom lecture, presentation to be intermixed with various types of interactive engagements.
- Power point presentation with interactive discussions
- Flipped classroom

Assessment Methods:

Apart from the regular assessment we are doing assignments, house examination we should also have a field trip or visit to any pharmaceutical company must be there for every semester and student should submit their report of that visit.

Keywords:

Alkyl halides, Alcohols, Phenols, Ethers, Carbonyl Compounds

CHEMISTRY - CVII: PHYSICAL CHEMISTRY–III

Phase Equilibria and Electrochemical Cells

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

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

Objectives:

1.Understand concepts of electrochemistry, batteries, phase, co-existence of phases, phase diagram, CST and distribution law.

2. Understand surface phenomenon, adsorption isotherms, BET Equation.

Learning Outcomes:

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

1. Explain the terms of electrochemistry, cell battery, corrosion and happenings in surroundings.
2. Explain phase equilibrium, criteria, CST, Gibbs-Duhem Margules Eqn

Unit 1:

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems (H2O and S), with applications. A comparison between the phase diagram of CO2 and H2O. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points. Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non ideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications.

(Lectures: 27)

Unit 2:

Electrochemical Cells: Rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry. Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb2O3 electrodes. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation).

(Lectures: 27)

Unit 3:

Surface chemistry: Physical adsorption, chemisorption, adsorption isotherms (Langmuir and Freundlich). nature of adsorbed state. Qualitative discussion of BET.

(Lectures: 06)

Practical:
(Credits: 2, Lectures: 60)

Phase Equibria:

1. Determination of critical solution temperature and composition at CST of the phenol water system and to study the effect of impurities of sodium chloride and succinic acid on it.
2. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method: a. simple eutectic and b. congruently melting systems.
3. Distribution of acetic/ benzoic acid between water and chloroform or cyclohexane.

4. Study of equilibrium of atleast one of the following reactions by distribution method:
    a. I_2 (aq) + I^- (aq) $\longrightarrow$ I_3^-(aq)
    b. Cu^{2+} (aq) + nNH_3 $\longrightarrow$ $[Cu(NH_3)_n]^{2+}$

Potentiometry:

1. Perform the following potentiometric titrations: i. Strong acid vs. strong base ii. Weak acid vs. strong base iii. Dibasic acid vs. strong base iv. Potassium dichromate vs. Mohr's salt

References:

- Peter Atkins & Julio De Paula, Physical Chemistry 9th Ed., Oxford University Press (2010).
- Castellan, G. W. Physical Chemistry, 4th Ed., Narosa (2004).
- McQuarrie, D. A. & Simon, J. D., Molecular Thermodynamics, Viva Books Pvt. Ltd.: New Delhi (2004).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- Zundhal, S.S. Chemistry concepts and applications Cengage India (2011).
- Ball, D. W. Physical Chemistry Cengage India (2012).
- Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
- Levine, I. N. Physical Chemistry 6th Ed., Tata McGraw-Hill (2011).
- Metz, C. R. Physical Chemistry 2nd Ed., Tata McGraw-Hill (2009).

Teaching Learning Process:

- Chalk and board should not be only method for teaching.
- Power point presentation, small Group discussion among students should be included, Chalk and board method is not student centric, methods should be included that make teaching more students centric and inclusive. This can be possible in a class of 40 to 45 students, more students make teaching teacher centric. Rote learning should be avoided. Different pedagogical tools are required to fulfill the same

Assessment Methods:

- One assignment for all students, one class test and attendance is not good criterion to assess the students . We should assess our students on regular basis not one time at the end of the semester.

Keywords:

SEMESTER IV

CHEMISTRY - CVIII: INORGANIC CHEMISTRY - III
Coordination Chemistry

Total Credits: 06 **(Credits: Theory-04, Practicals-02)**
(Total Lecture: Theory- 60, Practicals-60)

Objectives:

The course introduces the students to coordination compounds which find manifold applications in diverse areas like qualitative and quantitative analysis, metallurgy, as catalysts in industrial processes as medicines, paints and pigments as well as in life. The student is also familiarized with the d and f block elements and get an idea about horizontal similarity in a period in addition to vertical similarity in a group.

Learning Outcomes:

By the end of the course, the students will be-

On completion of the course the student will be able to:

1) Understand the terms, ligand, denticity of ligands, chelate, coordination number and use standard rules to name coordination compounds.
2) Discuss the various types of isomerism possible in such compounds and understand the types of isomerism possible in a metal complex.
3) Use Valence Bond Theory to predict the structure and magnetic behaviour of metal complexes and understand the terms inner and outer orbital complexes
4) Explain the meaning of the terms Δ_o., Δ_t, pairing energy, CFSE, high spin and low spin and how CFSE affects thermodynamic properties like lattice enthalpy and hydration enthalpy
5) Explain magnetic properties and colour of complexes on basis of Crystal Field Theory
6) Understand the important properties of transition metals like variable oxidation states, colour, magneticand catalytic properties and use Latimer diagrams to predict and identify species which are reducing, oxidizing and tend to disproportionate and calculate skip step potentials
7) Understand reaction mechanisms of coordination compounds and differentiate between kinetic and thermodynamic stability

---

Unit 1:

Coordination Chemistry:

Recapitulation of Werner's Coordination theory

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. with coordination numbers 4 and 6. A brief idea about chelate effect and labile and inert complexes.

Valence bond theory and its application to complexes of coordination numbers 4 and 6. Examples of inner and outer orbital complexes.

Crystal field theory, measurement of Δ_o. Calculation of CFSE in weak and strong fields, concept of pairing energies, factors affecting the magnitude of Δ_o. Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory (for octahedral sigma donor, π- acceptor and π- donor complexes)

(26 Lectures)

Unit 2:

Transition Elements: General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, and ability to form complexes.Latimer diagrams of Mn, Fe and Cu in acidic and basic media
A brief discussion of differences between the first, second and third transition series.
Some important compounds of Cr, Mn, Fe and Co and their roles as laboratory reagents;
Potassium dichromate, potassium permanganate, potassium ferrocyanide, potassium ferricyanide,, sodium nitroprusside and sodium cobaltinitrite.

(14 Lectures)

Unit 3:

Lanthanoids and Actinoids:A brief discussion of electronic configuration, oxidation states, colour, spectral and magnetic properties

Lanthanoid contraction (causes and effects) separation of lanthanoids by ion exchange method.

(6 Lectures)

Unit 4:

Inorganic Reaction Mechanism: Introduction to inorganic reaction mechanisms. Concept of reaction pathways, transition state, intermediate and activated complex Substitution reactions in square planarcomplexes, Trans- effect, theories of trans effect. Thermodynamic and Kinetic stability (using VBT)

(14 Lectures)

Practical:

(Credit: 2, Lab: 60 Lectures)

Objective

To correlate the theoretical concepts with practical applications in diverse fields

Learning outcomes

These experiments will develop skills of students and they will be able to

· Apply gravimetric analysis to determine composition of various sqamples including ores, alloys

· Prepare coordination properties and study their properties.

Gravimetry

Estimation of nickel (II) using dimethylglyoxime (DMG).
ii. Estimation of copper as CuSCN
iii. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.

iv. Estimation of Al(III) by precipitating with oxine and weighing as $Al(oxine)_3$
(aluminium oxinate).
Inorganic Preparations:
i. Tetraamminecopper (II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$
ii. Acetylacetonate complexes of Cu^{2+}/Fe^{3+}

iii. Potassium tri(oxalato)ferrate(III)
Properties of Complexes
i. Measurement of Δ_o. by spectrophotometric method
ii. Verification of spectrochemical series.
iii. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

References:

Theory:

- Atkins, P., & Overton, T. *Shriver and Atkins' inorganic chemistry 6th Ed.* Oxford University Press, USA, 2010.
- Pfennig, B. W. *Principles of inorganic chemistry*. John Wiley & Sons, 2015.
- Purcell, K.F & Kotz, J.C., Inorganic Chemistry W.B. Saunders Co, 1977.
- Huheey, J.E., *Inorganic Chemistry,* Prentice Hall, 1993.
- Cotton, F.A. & Wilkinson, G., *Advanced Inorganic Chemistry* Wiley-VCH, 1999
- Basolo, F, and Pearson, R.C., *Mechanisms of Inorganic Chemistry,* John Wiley & Sons, NY, 1967.
- Greenwood, N.N. & Earnshaw A., *Chemistry of the Elements,* Butterworth-Heinemann,1997.
- Miessler, G. L. &. Tarr, Donald A. *Inorganic Chemistry 3rd Ed.(adapted),* Pearson, 2009
- Barnes, C. E. *Inorganic Chemistry 4th Ed.* (Catherine E. Housecroft and Alan G. Sharpe). Journal of Chemical Education, 2003.

Practicals:

- Vogel, A.I. A text book of Quantitative Analysis, ELBS 1986.
- G. Marr and B.W. Rockett, Practical Inorganic Chemistry

CHEMISTRY - CIX: ORGANIC CHEMISTRY - III

Heterocyclic Chemistry

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

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

Objectives:

The Core Course Organic Chemistry III is infused with the details of Nitrogen containing functional groups and introduction of polynuclear hydrocarbons, heterocyclic systems and natural compounds *viz* terpenes and alkaloids. A comprehensive understanding of these topics will be developed by taking examples of 2-3 representatives members of each class. The chemical synthesis, properties and reactions of these compounds will be discussed in details. This course will also discuss some of the key applications of each class of compounds in diverse fields.

Learning Outcomes:

On completion of this course, the students will be able to do the following:

1. Gain theoretical understanding of chemistry of compounds having nitrogen containing functional groups, heterocyclics, polynuclear hydrocarbons, alkaloids and terpenes which includes various methods for synthesis through application of the synthetic organic chemistry concepts learnt so far.
2. Become familiar with their particular properties, chemical reactions, criterion of aromaticity with reference to polynuclear hydrocarbons and heterocyclic compounds, trends in basicity of amines and heterocyclics compounds and their behaviour at different pH.
3. Learn practical approach to structural elucidation of organic compounds with specific examples of terpenes and alkaloids.
4. Predict the carbon skeleton of amines and heterocyclic compounds via use of Hoffmann's exhaustive methylation and Emde's modification methods.
5. Understand the applications of these compounds including their medicinal applications through their reaction chemistry.

Unit 1:

Nitrogen Containing Functional Groups

Preparation, properties and important reactions of amines and diazonium salts, nitro compounds, nitriles and isonitriles.

A) Amines: Introduction, classification, chirality in amines (pyramidal inversion), importance and general methods of preparation.

Properties : Physical properties, Basicity of amines: Effect of substituent , solvent and steric effects. Distinction between Primary , secondary and tertiary amines using Hinsberg's method and nitrous acid. Discussion of the following reactions with emphasis on the mechanistic pathway: Gabriel Phthalimide synthesis, Hoffmann- Bromamide reaction, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction and Cope elimination.

Diazonium Salts: Preparation and synthetic applications of diazonium salts including preparation of arenes, haloarenes, phenols, cyano and nitro compounds. Coupling reactions of diazonium salts(preparation of azo dyes).

B) **Nitro compounds (**Aliphatic and Aromatic**)**:Nomenclature, classification and general methods of preparation: from alkyl halides, alkanes, oxidation of amines and oximes and diazonium salts.

Properties: Physical properties, discussion on the following reactions with mechanism:

Reaction with alkali and its synthetic applications, condensation reaction, Mannich reaction, Hydrolysis ,Reduction- electrolytic reduction, reduction in acidic, basic and neutral medium (for aromatic compounds) ,reaction with nitrous acid, Electrophilic substitution-Halogenation, nitration and sulphonation reaction, and Nucleophilic substitution on the ring .

C) Nitriles: Introduction, Nomenclature and uses. Preparation from the following reactions: Dehydration of amides and aldoximes, substitution reaction in alkyl halides and tosylates, from Grignard reagents and from dehydrogenation of primary amines.

Properties: Physical properties, discussion on the following reactions with mechanism:

Reaction with Grignard reagent, hydrolysis ,addition reaction with HX,NH_3 ,reaction with aqueous ROH, Reduction reactions-catalytic reduction and Stephen's reaction, Condensation reactions-Thorpe Nitrile Condensation.

D) Isonitriles: Introduction, Nomenclature and uses. Preparation from the following reactions:

Carbylamine reaction, substitution in alkyl halides and dehydrogenation of N-substituted formamides.

Properties: Physical properties, discussion on the following reactions with mechanism:

Hydrolysis, reduction, addition of – HX, X_2 and sulphur, Grignard reagent reaction, oxidation and rearrangement.

(18 Lectures)

Unit 2:

Polynuclear Hydrocarbons

Introduction, Classification ,Structure , Nomenclature and uses. Aromaticity of polynuclear hydrocarbons, structure elucidation of Naphthalene and general methods of preparation of naphthalene, phenanthrene and anthracene(Including Howarth method ,Friedel Craft acylation, Diels Alder reaction ,Elbs reaction and Pschorr Synthesis).Relative reactivity of naphthalene, phenanthrene and anthracene in comparison to benzene.

Properties: Physical properties, discussion on the following reaction (with mechanism) for Naphthalene, Anthracene and Phenanthrene:

Addition reactions, Oxidation, Electrophilic substitution- Friedel Craft reaction, Chloromethylation, Halogenation, Formylation, Nitration and sulphonation. Reduction reaction and Diels Alder reaction.

(8 Lectures)

Unit 3:

Heterocyclic Compounds

Introduction, importance, classification and nomenclature of heterocyclic compounds (containing only one hetero atom). General discussion on the following aspects of heterocyclic compounds: Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Basicity and relative reactivity towards electrophilic substitution reactions(amongst five membered and six membered rings)

General methods of synthesis for : Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Indole(Fischer indole synthesis and Madelung synthesis, reduction of o-nitrobenzaldehyde), Quinoline and isoquinoline, (Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner- Miller synthesis, Bischler-Napieralski reaction, PictetSpengler reaction, Pomeranz-Fritsch reaction)

Properties: Physical properties, discussion on the following reaction (with mechanism) for Furan, Pyrrole, thiophene, Pyridine, Indole , Quinoline and Isoquinoline: Electrophilic substitution- Nitration, sulphonation, halogenation, Formylation, acylation, mercuration and carboxylation. Oxidation ,Reduction, Addition, Reactions showing acidic /basic character.Reaction with diazonium salts, Ring opening, Ring expansion and Nucleophilic substitution reaction wherever applicable should be discussed

(22 Lectures)

Unit 4:

Alkaloids

Introduction, Natural occurrence, Classification, Uses, general structural features, general methods for structure elucidation including Hoffmann's exhaustive methylation and Emde's method. Structure elucidation, synthesis and physiological action of Nicotine.

(6 Lectures)

Unit 5:

Terpenes

Introduction, Occurrence, Uses, classification, isoprene and special isoprene rule; general methods of structure elucidation including distinction between isopropylidene and isopropenyl group, Elucidation of structure and synthesis of Citral ,its industrial application.

(6 Lectures)

Practical:

(Credits: 2, Lectures: 60)

1. Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols, carbonyl compounds and esters)
2. Isolation of caffeine from tea leaves.
3. Estimation of aniline by following methods :a) Acetylation b) Bromate-bromide method

References:

Theory:

- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd.
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Welly& Sons (1976). Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
- Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, PrajatiParakashan (2010).
- Thomas L. Gilchrist, Heterocyclic chemistry, Pearson Education, 3. ed. 1997 (ISBN 0-582-27843-0).

Practical:

- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
- Ahluwalia, V.K. &Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).

Teaching Learning Process:

The teaching learning process will involve the flipped classroom technique along with traditional chalk and black board method. Certain topics like pyramidal inversion, stereochemistry of Hoffman elimination and Cope elimination 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.

Assessment Methods:

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

Keywords:

Nitrogen containing functional groups, Polynuclear hydrocarbons, Heterocyclic compounds, Terpenes and Alkaloids, Synthetic Organic Chemistry.

CHEMISTRY - CX: PHYSICAL CHEMISTRY–IV

Conductance & Chemical Kinetics

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

Objectives:

1.This course aims to make the students understand laws governing migration of ions and use conductance as a tool to calculate important parameters.

2. To understand kinetics of chemical reaction, catalysis and photochemical reactions.

Learning Outcomes:

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

1. To understand the concept of ionic dissociation and types of electrolytes.
2. To learn about laws governing migration of ions in solutions, various ways of quantifying conductance and its experimental determination.
3. To be able to apply this knowledge in determining important parameters like solubility product, dissociation constants etc
4. To be able to define rate of reactions and the factors that affect the rates of reaction.
5. To understand the concept of rate laws e.g., order, molecularity, half life etc. and their determination.
6. To learn about various theories of reaction rates and how these account for experimental observations.
7. To be able to deduce rate laws from reaction mechanisms thereby grasping the concepts of elementary and complex reactions and chain reactions, steady state approximation and rate determining step.
8. To understand the mechanism of catalytic action on reactions for homogeneous, surface catalyzed and enzyme catalyzed reactions.
9. To learn about the laws of absorption of light energy by molecules and the subsequent photochemical reactions.
10. To understand the concept of quantum efficiency and mechanisms of photochemical reactions.

Unit 1:

Conductance: Quantitative aspects of Faraday's laws of electrolysis, Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rule. Ionic velocity, mobility and their determination, transference number and its relation to ionic mobility, determination of transference number using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations,(v) hydrolysis constants of salts.

(18 Lectures)

Unit 2:

Chemical Kinetics: Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods for determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i)

Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions. Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates.

(22 Lectures)

Unit 3:

Catalysis: Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis.

(8 Lectures)

Unit 4:

Photochemistry: Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence.

(12 Lectures)

Practical:

(Credits: 2, Lectures: 60)

Conductometry

1. Determination of cell constant
2. Determination of conductivity, molar conductivity, degree of dissociation and dissociation constant of a weak acid.
3. Perform the following conductometric titrations: i. Strong acid vs. strong base ii. Weak acid vs. strong base iii. Mixture of strong acid and weak acid vs. strong base, strong acid vs. strong base.

Chemical Kinetics:

1. To study the kinetics of Acid hydrolysis of methyl acetate with hydrochloric acid using integrated rate law method.
2. To study the kinetics of Iodide-persulphate reaction by Initial rate method.
3. To study the kinetics of iodine-persulphate reaction using integrated rate law method.
4. To study the kinetics of Saponification of ethyl acetate.

References:

Theory:

1. Atkins, P.W & Paula, J.D. Physical Chemistry, 10th Ed., Oxford University Press (2011).
2. Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
3. Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed., John Wiley & Sons, Inc. (2005).
4. Kapoor, K.L. A Textbook of Physical Chemistry, McGraw Hill Education (India) (2014)

5. Ball, D,W. Physical Chemistry, Cengage India Private Limited 2nd Ed.(2017)
6. Laidler K.J. Chemical Kinetics 3rd Ed. Pearson Education India(2003)

Additional Resources:

1. Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
2. Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
3. Barrow, G. M., Physical Chemistry 5th Ed., Tata McGraw Hill: New Delhi (2006).
4. Rogers, D. W. Concise Physical Chemistry Wiley (2010).
5. Glasstone, S. Textbook of Physical Chemistry, Mcmillan,,Canada (1948)

Practicals:

1. Khosla, B.D., Garg, V.C. and Gulati, A. Senior Practical Physical, R.Chand & Co., New Delhi (2011).

Teaching Learning Process:

1. Interactive teaching methods to be used. Each topic to be presented by the teacher. Multimedia may be used wherever possible if it enhances the quality of presentation e,g., where 3 D visualization is required.
2. Conceptual and numerical problems should be discussed in the class and active participation of students should be encouraged.
3. Group work may be introduced. The class is divided into groups of 3-4 students. Each group is given a problem which they discuss and solve and present the solution to the class. This may be followed by the whole class participating in the discussion.
4. In lab work the students should be told beforehand about the experiment to be performed. They are expected to come prepared with the conceptual and procedural part of the experiment. This can then be discussed before start of the practical. Special emphasis should be on sources of error and results of all students/groups may be compared in the end.

Assessment Methods:

1. Frequent short quiz testing conceptual understanding.
2. Open book assignments to be completed in class.
3. Group presentation as discussed in teaching - learning methods may be used for assessment.
4. In lab work assessment should be based on following

   a. Conceptual understanding
   b. Presentation of data
   c. Internal consistency
   d. Result (taking into consideration the unavoidable errors)

Keywords:

Conductance, Transference Number, Rate law, Order. Elementary and Complex Reactions, Reaction mechanism, Steady state Principle. Activation Energy, Catalyst, Quantum Efficiency.

SEMESTER V

CHEMISTRY - CXI: ORGANIC CHEMISTRY - IV

Biomolecules

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

(Total Lecture: Theory- 60, Practicals-60)

Objectives:

The core course of Organic Chemistry IV is an extrapolation of fundamental concept and functional group chemistry studied in the previous core courses. The focus area of this course is on the chemistry of biomolecules i.e. amino acids, peptides, proteins, enzymes, carbohydrates and lipids. Through the study of energetics in biological systems, it aims to build the concept of metabolism for biological systems more lucid.

Learning Outcomes:

On completion of this course, the students will be able to do the following:

1. Understand and demonstrate how structure of biomolecules determines their reactivity and biological functions
2. Gain insight into concepts of heredity through the study of genetic code, replication, transcription and translation.
3. Demonstrate and understanding of metabolic pathways, their inter relationship, regulation and energy production from biochemical processes.

Unit 1:

Nucleic acids:

Structure of components of nucleic acids: Bases, Sugars, Nucleosides and Nucleotides. Nomenclature of nucleosides and nucleotides, structure of polynucleotides (DNA and RNA), Biological roles of DNA and RNA. Concept of heredity:Genetic Code, Replication, Transcription and Translation.

(9 Lectures)

Unit 2:

Amino Acids, Peptides and Proteins:

Amino acids, Peptides and their classification. α-Amino Acids - Synthesis, ionic properties and reactions. Zwitterions, pKa values, isoelectric point and electrophoresis; Study of peptides: determination of their primary structures-end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups, Solid-phase synthesis; primary, secondary and tertiary structures of proteins, Denaturation

(**18 Lectures**)

Unit 3:

Enzymes

Introduction, classification and characteristics of enzymes. Salient features of active site of enzymes. Mechanism of enzyme action (taking chymotrypsin as an example), factors affecting enzyme action, coenzymes and cofactors (NAD,FAD), specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance.

(7Lectures)

Unit 4:

Carbohydrates

Occurrence, classification and their biological importance. Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures; 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.

(**18 Lectures**)

Unit 5:

Concept of energy in biosystems

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 carbohydrate- glycolysis, fermentation, Krebs cycle. Caloric value of food, standard caloric content of food types.

(**9Lectures)**

Practical:
(Credits: 2, Lectures:60)

1.Estimation of glycine by Sorensen formol method.
2.Study of the titration curve of glycine.
3.Estimation of proteins by Lowry's method.
4.Study of the action of salivary amylase on starch under optimum conditions.
5.Effect of temperature on the action of salivary amylase.
6. Isolation and estimation of DNA using cauliflower/onion.

References:

Theory:

•Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) Biochemistry. VIth Edition. W.H. Freeman and Co.
•Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) Principles of Biochemistry. IV Edition. W.H. Freeman and Co.
•Murray, R.K., Granner, D.K., Mayes, P.A. and Rodwell, V.W. (2009) Harper's Illustrated Biochemistry. XXVIII edition.Lange Medical Books/McGraw-Hill.

Practical:

- Manual of Biochemistry workshop, 2012, Department of Chemistry, University of Delhi.
- Introduction to Practical Biochemistry by Randhir Singh and S. K. Sawhney, Nerosa Publications.

Additional Resources:

Finar,I.L. (2008) Organic Chemistry, Volume 2, Fifth Edition, Pearson Education

Teaching Learning Process:

- Teaching Learning Process for the course is visualized as largely student- focussed.
- Transaction through an intelligent mix of conventional and modern methods
- Frequent use of molecular models for demonstration and providing students in groups to explore building models themselves
- engaging students in cooperative learning
- learning through quiz design
- Problem solving to enhance comprehension

Assessment Methods:

- Graded assignment
- Conventional class tests
- Class seminars by students on course topics with a view to strengthening the content through width and depth
- Quizzes
- Term Papers

Keywords:

Amino acids, peptides, proteins, solid phase peptide synthesis, Killiani- Fischer synthesis, Amadori rearrangement, Lobry de Bruyn van Ekenstein rearrangement, Saponification value, Iodine number, rancidity, reversion, Krebs cycle, Glycolysis, Enzymes, inhibitors

---

CHEMISTRY - CXII: PHYSICAL CHEMISTRY–V
Quantum Chemistry & Spectroscopy

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

Objectives:

1. The objective of this course is to identify the limitations of classical mechanics and the need of quantum chemistry.
2. To familiarize the students with postulates of quantum chemistry and apply them to derive equations for various models and hydrogen atoms.

Learning Outcomes:

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

1. Inadequacy of classical mechanics to deal with microscopic systems.
2. Relation between observables and quantum mechanical operators.
3. Concepts of boundary conditions and quantization, probability distribution, most probable values, uncertainty and expectation values.
4. Application of quantization to spectroscopy.
5. Various types of spectra and their use in structure determination.

Unit 1:

Quantum Chemistry: Postulates of quantum mechanics, quantum mechanical operators and commutation rules, Schrödinger equation and its application to free particle and particle in a box (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wave functions, probability distribution functions, nodal properties, Extension to two and three dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation in Cartesian and spherical polar (Derivation not required). Separation of variables. Spherical harmonics. Discussion of solution (Qualitative).

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part and quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

(22 Lectures)

Unit 2

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAOMO treatment of H_2^+. Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H_2 (only wave functions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH).

(8 Lectures)

Unit 3

Molecular Spectroscopy: Interaction of electromagnetic radiation with molecules and various types of spectra; Born Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies.

Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales (δ and T), spin-spin coupling and high resolution spectra, interpretation of PMR spectra of simple organic molecules like methanol, ethanol, acetaldehyde, acetic acid and aromatic proton.

Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

(30 Lectures)

Practical:
(Credits: 2, Lectures: 60)

Colorimetry :

1. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration.
2. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
3. Study the kinetics of iodination of propanone in acidic medium.

4. Determine the amount of iron present in a sample using 1, 10-phenathroline.
5. Determine the dissociation constant of an indicator (phenolphthalein).

6. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

Spectrophotometry:

1.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 (kJ molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
4. Analysis of the given vibration-rotation spectrum of HCl(g)

References:

Theory:

- Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).
- Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press (2005).
- House, J.E. Fundamentals of Quantum Chemistry, 2nd Ed. Elsevier, USA (2004)
- McQuarrie, D.A. Quantum Chemistry, Viva Books (2016)
- Prasad, R.K. Quantum Chemistry, New Age (2010)

Practical:

- Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co. New York (2003).

Additional Resources:

- Chandra, A. K. Introductory Quantum Chemistry Tata McGraw-Hill (2001).
  Kakkar, R. Atomic & Molecular Spectroscopy, Cambridge University Press (2015).
- Engel, T. and Reid, P., Quantum Chemistry and Spectroscopy, Pearson, (2013)
- Aruldhas, G. Quantum mechanics,2nd Ed., Prentice Hall India Learning Pvt. Ltd., (2008)
- Bockhoff,F.J., Elements of Quantum Theory, Addison – Wesley Publishing Company, (1969)
- Ponomarev, L.I., The quantum Dice, CRC Press(1993)
- Gamow,G., Mr. Tompkins, Cambridge University Press, (2012)

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:

There should be a multi-pronged approach for evaluating a student's understanding of the key concepts. Some of the methods that can be used are:

- Class assignments
- Short quiz
- Presentations

Keywords:

Schrodinger equation, Quantum Number, selection rules, approximation methods, molecular orbital, MO Diagram, pi bond, spectrum, rotation, vibration, resonance.

SEMESTER VI

CHEMISTRY - CXIII: INORGANIC CHEMISTRY - IV
Organometallic Chemistry & Bio-inorganic Chemistry

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

Objectives:

The course introduces some important topics of Inorganic Chemistry in a compact way. Unit 1 of the course introduces students to the basic principles of qualitative inorganic analysis. The influence of solubility products and the common ion effect on the separation of cations is made clear. Interfering anions are identified and their removal studied. Unit 2 an introduction to the very important area of Organometallic Chemistry including classification of organometallic compounds, the concept of hapticity and the 18-electron rule governing the stability of a wide variety of organometallic species. Specific organometallic compounds are studied in detail to further understand the basic concepts: metal carbonyls, metal alkyls, Zeise's salt and ferrocene. Unit 4 takes this a step further by covering Catalysis, an important application of organometallic compounds. Under Unit 3, Bioinorganic Chemistry, the student learns the importance of inorganic chemical species, especially metals, in biological systems, through discussions on metal-containing enzymes, the sodium-potassium pump and the applications of iron in physiology, including iron transport and storage system.

Learning Outcomes:

By the end of the course, the students will be-

1. Understand and explain the basic principles of qualitative inorganic analysis
2. Apply the concepts of solubility product and common ion effect to the separation of cations and anions including choice of group reagent (under H_2S scheme) for separation of cations into groups
3. Define and classify organometallic compounds and explain the concept of hapticity of ligands.
4. Apply 18-electron rule to rationalize the stability of metal carbonyls and related species and describe the general methods of preparation and structures of mono and binuclear carbonyls of 3d series
5. Describe the preparation and structure of Zeise's salt and compare the synergic effect of carbonyls and Zeise's salt and correlate IR data to the extent of back bonding
6. Identify important structural features of the metal alkyls tetrameric methyl lithium and dimeric trialkyl aluminium and explain the concept of multicenter bonding in these compounds
7. Diagrammatically explain the working of the sodium-potassium pump in organisms and the factors affecting it and understand and describe the active sites and action cycles of the metalloenzymes carbonic anhydrase and carboxypeptidase
8. Explain the sources and consequences of excess and deficiency of trace metals and learn about the toxicity of certain metal ions, the reasons for toxicity and antidotes
9. Explain the use of chelating agents in medicine and, specifically, the role of cisplatin in cancer therapy and explain the applications of iron in biological systems with particular reference to haemoglobin, myoglobin, ferritin and transferrin
10. Get a general idea of catalysis and describe in detail the mechanism of the following processes: alkene hydrogenation with Wilkinson's catalyst, polymerization of ethene using Ziegler-Natta catalyst, synthetic gasoline manufacture by Fischer-Tropsch process.

Unit 1:

Theoretical Principles in Qualitative Analysis (H_2S Scheme)

Basic principles involved in analysis of cations and anions. Solubility products, common ioneffect. Principles involved in separation of cations into groups and choice of group reagents.Interfering anions (fluoride, borate, oxalate and phosphate), need to remove them afterGroup II and methods of removal. Analysis of insoluble substances.

(12 Lectures)

Unit 2:

Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds.

Ferrocene: Preparation, physical properties and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

(22 Lectures)

Unit 3:

Bioinorganic Chemistry:

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine, Cisplatin as an anti-cancer drug.

Iron and its application in bio-systems, Haemoglobin, Myoglobin; Storage and transfer of iron.

(18 Lectures)

Unit 4:

Catalysis by Organometallic Compounds:

General principles of catalysis, properties of catalysts, homogeneous and heterogeneous catalysis (catalytic steps, examples and industrial applications), deactivation and regeneration of catalysts, catalytic poison, promoter.

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinson's Catalyst)

2. Synthetic gasoline (Fischer Tropsch reaction)

3. Polymerisation of ethene using Ziegler-Natta catalyst

(8 Lectures)

Practical:

Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-},$S_2O_3^{2-}$, CH_3COO^-, F^-,Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}

Mixtures should preferably contain one interfering anion, or insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) or combination of anions e.g. CO_3^{2-} and SO_3^{2-}, NO_2^- and NO_3^-, $Cl^-$and Br^-, Cl^- and I^-, Br^- and I^-, NO_3^- and Br^-, NO_3^- and I^-. Spot tests should be done whenever possible.

References:

Theory:

- Vogel, A.I. *Qualitative Inorganic Analysis,* Longman, 1972
- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall,1996-03-07.

Practical:

- Cotton, F.A., Wilkinson, G., & Gaus, P.L. *Basic Inorganic Chemistry 3rd Ed.;*Wiley India,Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed.,* Harper Collins 1993, Pearson 2006.
- Sharpe, A.G. *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005
- Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry3rd Ed.,* John Wiley and Sons, NY, 1994.
- Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements 2nd Ed,* Elsevier, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
- Lee, J.D. *Concise Inorganic Chemistry 5th Ed.,* John Wiley and sons 2008.
- Powell, P. *Principles of Organometallic Chemistry*, Chapman and Hall, 1988.
- Shriver, D.D., Atkins, P. and Langford, C.H., *Inorganic Chemistry 2nd Ed.,* Oxford University Press, 1994.
- Purcell, K.F. & Kotz, J.C., *Inorganic Chemistry*, W.B. Saunders Co. 1977

Additional Resources:

- Lippard, S.J. & Berg, J.M., *Principles of Bioinorganic Chemistry* Panima Publishing Company 1994.
- Miessler, G. L. & Tarr, Donald A., *Inorganic Chemistry 4th Ed.,* Pearson, 2010.
- Collman, James P. et al. *Principles and Applications of Organotransition Metal Chemistry.* Mill Valley, CA: University Science Books, 1987.
- Crabtree, Robert H. *The Organometallic Chemistry of the Transition Metals*. John Wiley New York, NY, 2000.
- Spessard, Gary O., & Miessler, Gary L., *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.

Keywords:

Qualitative analysis; solubility products; common ion effect; interfering anion; Organometallic Compounds; carbonyls; 18-electron rule; synergic bonding; IR spectra of carbonyls; Zeise's salt; metal alkyls; ferrocene; Bioinorganic Chemistry; sodium-potassium pump; carboxypeptidase; carbonic anhydrase; haemoglobin and myoglobin; trace metals; metal toxicity; chelates in medicine; cisplatin; homogeneous and heterogeneous catalysis; Ziegler Natta catalyst; Wilkinson's catalyst; Fischer Tropsch process; ZSM 5

CHEMISTRY - CXIV: ORGANIC CHEMISTRY - V

Spectroscopy

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

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

Objectives:

The core course of Organic Chemistry V deals with some classes of organic compounds finding applications in everyday life namely; polymers, dyes, lipids and pharmaceutical compounds. The chemistry of these compounds in general will be explained through naturally occurring and synthetic compounds. The course also introduces the learner to various tools and techniques for identifying and characterizing the organic compounds through their interactions with electromagnetic radiation viz. IR, NMR and UV- Visible spectroscopy.

Learning Outcomes:

On completion of this course, the students will be able to do the following:

1. Gain insight into the basic principles of NMR, IR and UV spectroscopic techniques.
2. Learn to apply the principles to find out the structure of unknown organic molecules and in determination of their stereochemistry.
3. Develop a sound understanding of the structure of Pharmaceutical Compounds. They will also understand the importance of different classes of drugs and their applications for treatment of various diseases.
4. Learn about the chemistry of natural and synthetic polymers including fabrics and rubbers.
5. Understand the chemistry of biodegradable and conducting polymers and appreciate the need of biodegradable polymers with emphasis on basic principles.
6. Learn about the theory of colour and constitution as well as the chemistry of dyeing.
7. Able to know applications of various types of dyes including those in foods and textiles.

Unit 1:

Organic Spectroscopy

General principles Introduction to absorption and emission spectroscopy.
UV Spectroscopy: Types of electronic transitions, λmax, Chromophores and Auxochromes,Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of WoodwardRules for calculation of λmax for the following systems: α,β-unsaturated aldehydes, ketones,carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular;Extended conjugated systems (aldehydes, ketones and dienes);distinction between cis and trans isomers by UV.
IR Spectroscopy: Fundamental and non-fundamental molecular vibrations; IR absorptionpositions of O, N and S containing functional groups; Effect of H-bonding, conjugation,resonance and ring size on IR absorptions; Fingerprint region and its significance; application of IR in functional group analysis.
NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin – Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpretation of NMR spectra of simple compounds. Applications of IR, UV and NMR for identification of simple organic molecules.

(24 Lectures)

Unit 2:

Lipids

Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenation of fats and oils, Saponification value, acid value, iodine number. Reversion and rancidity.

(6 Lectures)

Unit 3:

Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing;

Synthesis and applications of Azo dyes – Methyl orange, Congo red; Triphenyl methane dyes -Malachite green, Rosaniline and Crystal violet; Phthalein Dyes – Phenolphthalein; Natural dyes –Structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

(8 Lectures)

Unit 4:

Pharmaceutical Compounds

Classification, structure and therapeutic uses of antipyretics - Paracetamol (with synthesis);Analgesics - Ibuprofen (with synthesis); Antimalarials - Chloroquine (with synthesis); Antitubercular drugs - Isoniazid. An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

(10 Lectures)

Unit 5:

Polymers

Introduction and classification including di-block, tri-block and amphiphilic polymers; weight average molecular weight, number average molecular weight, glass transition temperature (Tg) of polymers**;**Polymerisation reactions -Addition and condensation. Mechanism of cationic, anionic and free radical addition polymerization; Ziegler-Natta polymerisation of alkenes. Preparation and applications of plastics – thermosetting (phenol-formaldehyde, Polyurethanes) and thermosoftening (PVC, polythene); Fabrics – natural and synthetic (acrylic, polyamide, polyester). Rubbers – natural and synthetic, Buna-S, Chloroprene and Neoprene. Vulcanization - Polymer additives; Introduction to Biodegradable and conducting polymers with examples.

(12 Lectures)

Practical:
(Credits: 2, Lectures:60)

1. Qualitative analysis of unknown organic compounds containing monofunctional groups: aromatic hydrocarbons, aryl halides, carbohydrates, nitro compounds, amines, amides and simple compounds containing bifunctional groups, e.g. salicylic acid, cinnamic acid, nitrophenols.
2. Identification of simple organic compounds by IR and NMR spectroscopy(Spectra to be provided).
3. Quantitative analysis
   a. Saponification value of the given oil
   b. Iodine value of the given oil

References:
Theory:

- Pavia, D.L. Introduction to Spectroscopy, Cengage learning (India) Pvt. Ltd
- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
- Gowariker, V. R.; Viswanathan, N. V. &Sreedhar, J. Polymer Science, New Age International(P) Ltd. Pub.

- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of NaturalProducts), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- Kemp, W. Organic Spectroscopy, Palgrave
- Spectrometric Identification of Organic Compounds By Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce

Practical:

- Vogel, A.I. Quantitative Organic Analysis, Part 3, Pearson (2012).
- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry,
- 5th Ed., Pearson (2012)
- Ahluwalia, V.K. &Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- Ahluwalia, V.K. &Dhingra, S. Comprehensive Practical Organic Chemistry: QualitativeAnalysis, University Press (2000).

Additional Resources:

- Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
- Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, PrajatiPrakashan (2010).
- Billmeyer, F. W. Textbook of Polymer Science, John Wiley & Sons, Inc.

Teaching Learning Process:

- Conventional chalk and board teaching,
- Class interactions and discussions
- Showing 3D models of drugs and dyes using Chemdraw
- Power point presentation on important topics.

Assessment Methods:

- Presentations by Individual Student/ Small Group of Students
- Class Tests at Periodic Intervals.
- Written assignment(s)
- Objective type Chemical quizes based on contents of the paper.
- End semester University Theory and Practical Examination

Keywords:

CHEMISTRY DISCIPLINE ELECTIVE COURSES (DSE)

Novel Inorganic Solids

Chemistry - DSE 1 (i)
Total Credits: 06 **(Credits: Theory-04, Practicals-02)**
(Total Lectures: Theory- 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 have 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.

Course Learning Outcomes:

By the end of the course, the student would be able to:

(i) Understand the mechanism of solid-state synthesis.
(ii) Explain about the different characterization techniques and their principle.
(iii) Understand the concept of nanomaterials, their synthesis and properties.
(iv) Explain the mechanism of growth of self-assembled nanostructures.
(v) Appreciate the existence of bioinorganic nanomaterials.
(vi) Explain the importance of composites, conducting polymers and their applications.
(vii) Understand the usage of solid materials in various instruments, batteries, etc. which help them to appreciate the real life importance of these materials

Unit 1:

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

Synthesis and modification of inorganic solids: Conventional heat and beat method, Co-precipitation method, Sol-gel method, Hydrothermalmethod, Ion-exchange and Intercalation method.

(10 Lectures)

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)

(10 Lectures)

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.

(10 Lectures)

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.

(10 Lectures)

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.

(10 Lectures)

Unit 6:

Speciality polymers:

Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene, polyaniline

and polypyrole, 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.

(10 Lectures)

Practical:

(Credits: 2, Lectures: 60)

CHEMISTRY PRACTICAL - DSE LAB: 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

- West, A. R., Solid State Chemistry and Its Application, Wiley
- West, A. R., Application of Solid State Chemistry, Wiley
- Smart, L. E., Moore, E. A., Solid State Chemistry An Introduction CRC Press Taylor & Francis.
- Rao, C. N. R., Gopalakrishnan, J. New Direction of Solid State Chemistry, Cambridge University Press.
- Atkins, Peter, Overton, Tina, Rourke, Jonathan, Weller, Mark and Armstrong, Fraser *Shriver & Atkins' Inorganic Chemistry, 5th Edition*, Oxford University Press 2011-2012
- Adam, D.M. *Inorganic Solids: An introduction to concepts in solid-state structural chemistry,* John Wiley and Sons, London, New York, Sydney, Toronto, 1974
- Poole Jr., Charles P., Owens, Frank J., *Introduction to Nanotechnology* John Wiley and Sons, 2003.

Practical

- W. Orbaek, M. M. McHale, A. R. Barron, synthesis and characterization of silver nanoparticles for an undergraduate laboratory J. Chem. Educ. 2015, 92, 339−344.
- G. MacDiarmid, J. C. Chiang, A. F. Richter, N. L. D. Somasiri, Polyaniline: synthesis and characterization of the emeraldine oxidation state by elemental analysis. L. Alcaeer (ed.), Conducting Polymers, 105-120, 1987, D. Reidel Publishing.
- Industrial Inorganic Pigments edited by Gunter Buxbaum, Wiley-VCH
- K. H. Cheng, A. J. Jacobson, M. S. Whittingham, Hexagonal tungsten trioxide and its intercalation chemistry, Solid State Ionics, 5, 1981, 355-358.

· Ghorbani H. R, Mehr F. P, Pazoki H, Rahmani B. M. Synthesis of ZnO Nanoparticles by Precipitation Method. Orient J Chem 2015;31(2).
· D. J. Williams, B. E. Huck, A. P. Wilkinson, First-Year Undergraduate Laboratory Experiments with Zeolites, Chem. Educator 2002, 7, 33–36 33

Additional Resources:

https://www.youtube.com/watch?v=RuyP9kqRcLg

https://www.youtube.com/watch?v=BGPaywY1wvs

https://www.youtube.com/watch?v=x5OD2KZXd54

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:

Written Examination, Presentations, Quiz

Keywords:

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

Inorganic Materials of Industrial Importance

(CHEMISTRY DSE-1 (i)

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

1. Give the composition and applications of the different kinds of glass.
2. Understand glazing of ceramics and the factors affecting their porosity.
3. Give the composition of cement and discuss the mechanism of setting of cement.
4. Explain the suitability of fertilizers for different kinds of crops and soil.
5. Explain the process of formulation of paints and the basic principle behind the protection offered by the surface coatings.
6. Explain the principle, working and applications of different batteries.
7. List and explain the properties of engineering materials for mechanical construction used in day to day life.
8. 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: 08)

Unit 5:

Batteries:**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: 08)

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: 06)

Practical:

(Credits: 2, Lectures: 60)

PRACTICALS-DSE 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 Complexomety, 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:

- West, A. R., Solid State Chemistry and Its Application, Wiley
- Smart, L. E., Moore, E. A., Solid State Chemistry An Introduction CRC Press Taylor & Francis.
- Rao, C. N. R., Gopalakrishnan, J. New Direction of Solid State Chemistry, Cambridge University Press.
- Felder, R. M. and Rousseau, R.W., Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi, 2005.
- Atkins, Peter, and Tina Overton. Shriver and Atkins' inorganic chemistry. Oxford University Press, USA, 2010.
- Kingery, W. D., Bowen H. K. and Uhlmann, D. R. Introduction to Ceramics, Wiley Publishers, New Delhi, 1976.
- Kent, J. A. (ed) Riegel's Handbook of Industrial Chemistry, 9 th Ed., CBS Publishers, New Delhi, 1997
- Jain, P. C. and Jain, M. Engineering Chemistry, Dhanpat Rai & Sons, Delhi 2015
- Gopalan, R., Venkappayya, D. and Nagarajan, S. Engineering Chemistry, Vikas Publications, New Delhi, 2004.
- Sharma, B. K. Engineering Chemistry, Goel Publishing House, Meerut, 2015
- Mukhopadhyay R. and Datta S., Engineering Chemistry,New Age International(P) Ltd.,Publishers, (2010)

Practical:

- Vogel, Arthur I: A Text book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman.
- Svehl a, G., Vogel's Qualitative Inorganic Analysis 7th Ed., Prentice Hall, 1996.
- J. J. Banewicz, and C. T. Kenner, Determination of Calcium and Magnesium in Limestones and Dolomites, Anal. Chem., 1952, 24 (7), 1186–1187.
- Ghorbani H. R, Mehr F. P, Pazoki H, Rahmani B. M. Synthesis of ZnO Nanoparticles by Precipitation Method. Orient J Chem 2015;31(2).
- W. Orbaek, M. M. McHale, A. R. Barron, synthesis and characterization of silver nanoparticles for an undergraduate laboratory J. Chem. Educ. 2015, 92, 339−344.

Additional Resources:

https://www.youtube.com/watch?v=RuyP9kqRcLg

https://www.youtube.com/watch?v=BGPaywY1wvs

https://www.youtube.com/watch?v=x5OD2KZXd54

Teaching Learning Process:

Blackboard , Power point presentations, Assignments, Field Trips to Industry

Assessment Methods:

- Written Examination
- Presentations
- Quiz

Keywords:

Silicates, Ceramics, Cement, Fertilizers, Surface Coatings, Batteries, Engineering materials for mechanical construction**,** Nano Dimentional Materials

---

Applications of Computers in Chemistry

Chemistry DSE 2-4(i)

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

Objectives:

The aim of the paper is to make the students of chemistry familiar with the working of computer,programming language, QBASIC and use of software as a tool to understand chemistry, and solve chemistry based problems.

Learning Outcomes:

After completing the course the student should 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
3. Write BASIC programs for performing calculations involved in laboratory experiments and research work.
4. Use various spreadsheet software to perform 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, hyperchem, etc.), internet application.

(5 Lectures)

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 Waal 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).

(40 Lectures)

Unit 3:

Use of Software Products

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

(15 Lectures)

Practical:
(Credits: 2, Lectures: 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,Compressibilty 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:

- McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
- Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
- Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- Yates, P. Chemical Calculations. 2nd Ed. CRC Press (2007).

- Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis,Cambridge Univ. Press (2001)
- Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985).
- Venit, S.M. Programming in BASIC: Problem solving with structure and style Jaico Publishing House: Delhi (1996).

Teaching Learning Process:

Since the course involves programming and use of software, the teaching learning process becomes more efficient when the theory classes are well coordinated with practical exercises. Once the students learn BASIC commands, they may be encouraged to make their own programs.
QBASIC is a DOS based language which does not run on 64 bits Windows and Linux based operating systems. This problem can be solved by using DOSBOX emulator for different operating systems and running QB45 in it.
Another version which 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

---

Analytical Methods in Chemistry

Chemistry DSE 2-4(ii)

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

Objectives:

The objective of this course is to make student aware of the:

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

Learning Outcomes:

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

1. How to perform experiment with accuracy and precision.
2. Develop methods of analysis for different samples independently.
3. Test contaminated water samples.
4. Understand basic principle of instrument like Flame Photometer,UV-VISIBLE.
5. Learn separation of analytes by chromatography.
6. Apply knowledge of geometrical isomers and keto-enol tautomers to analysis.
7. How to determine composition of soil.
8. Estimation of macro nutrients using Flame photometry1

Unit 1:

Qualitative and quantitative aspects of analysis:
Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression.
Normal law of distribution of indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

(**5 Lectures)**

Unit 2:

Optical methods of analysis

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

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

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

Flame Atomic Absorption and Emission Spectrometry:
Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of

chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

(25 Lectures)

Unit 3

Thermal methods of analysis:
Theory of thermogravimetry (TG), basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture.

(**Lectures:05)**

Unit 4:

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

(**Lectures:10)**

Unit 5:

Separation techniques:

Solvent extraction:
Classification, principle and efficiency of the technique.
Mechanism of extraction: extraction by solvation and chelation, Technique of extraction: batch, continuous and counter current extractions, Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and non-aqueous media.

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

(Lectures:15)

Practical:

(Credits: 2, Lectures: 60)

I. Separation Techniques
Chromatography:
(a) Separation of mixtures
(i) Paper chromatographic separation of Co^{2+} and Ni^{2+}.
(ii) Separation and identification of the amino acids present in the given mixture by paper chromatography. Reporting the Rf values.
II. Solvent Extractions:
(i) To separate a mixture of Ni^{2+} & Fe^{2+} by complexation with DMG and extracting the Ni^{2+} DMG complex in chloroform, and determine its concentration by spectrophotometry.

Analysis of soil:
(i) Determination of pH of soil.
(ii) Total soluble salt
(iii) Estimation of calcium, magnesium
(iv) Qualitative detection of nitrate, phosphate
Ion exchange:
(i) Determination of exchange capacity of cation exchange resins and anion exchange resins.
(ii) Separation of amino acids from organic acids by ion exchange chromatography.
III Spectrophotometry
Verification of Lambert-Beer's law and determination of concentration of a coloured species ($CuSO_4$, $KMnO_4$)

References:

Theory:

- Vogel, Arthur I: A Text book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5 th Ed. The English Language Book Society of Longman .
- Willard, Hobart H. et al.: Instrumental Methods of Analysis, 7 th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6 th Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A., Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore, 1998.
- Mikes, O. and Chalmers, R.A. Ed. Laboratory Hand Book of Chromatographic and Allied Methods, Elles Horwood Ltd. London.
- Dilts, R.V. Analytical Chemistry – Methods of separation Van Nostrand 1974

Practical:

Vogel, Arthur I: *A Text book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5thEd. The English Language Book Society of Longman .
• Willard, Hobart H. et al.: *Instrumental Methods of Analysis, 7th Ed*. Wardsworth Publishing Company, Belmont, California, USA, 1988.
• Christian, Gary D; *Analytical Chemistry, 6th Ed*. John Wiley & Sons, New York, 2004.
• Harris, Daniel C: *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman, 2001.
• Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age, International Publisher, 2009.
• Skoog, D.A. Holler F.J. and Nieman, T.A. *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore, 1998.
• Mikes, O. & Chalmers, R.A. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Horwood Ltd. London.

Teaching Learning Process:

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

Assessment Methods:

- Presentations by Individual Student/ Small Group of Students
- Class Tests at Periodic Intervals.
- Written assignment(s)
- Objective type Chemical quizes based on contents of the paper.
- End semester University Theory and Practical Examination

Keywords:

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

Molecular Modelling and Drug Design

(Chemistry DSE2-4(iii)

Total Credits: 06 **(Credits: Theory-04, Practicals-02)**

(Total Lectures: Theory- 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:

Able to understand theoretical background of computational techniques, selective application to various molecular systems, draw energy minimization, ESP Plots by suitable softwares, electron rich and electron deficient sites, compare computational and experimental results and explain deviations.

Unit 1:

Introduction: Overview of Classical and Quantum Mechanical Methods (Ab initio, Semi-empirical, Molecuar 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 (5 classes)

(Lectures: 06)

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. Intermolecualr Potentials (Hard sphere, finite square well and Lennar-Jones potentials). 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 etc.

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 etc).

(Lectures: 8)

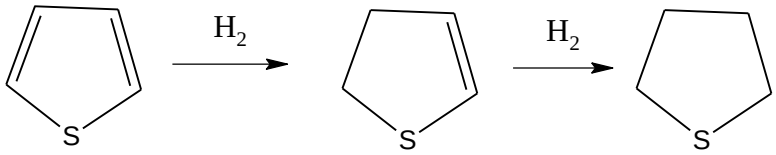
Practicals:

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 = CH3NH2, (CH3)2NH, (CH3)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 Arguslab.

Note: Software: ArgusLab (www.planaria-software.com).
Recommended Texts:

References:

Theory:

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

Practicals:

1. Lewars, E. G. Computational Chemistry 2nd Ed., Springer (India) Pvt. Ltd. 2011, Ch. 1 & 2.
2. Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall 2012, Ch. 26.

Keywords:

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

Chemistry - DSE 2-4 (iv)

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

1. Know about history of polymeric materials and their classification
2. Learn about different mechanisms of polymerization and also polymerization techniques
3. Evaluate kinetic chain length of polymers based on their mechanism
4. Differentiate between polymers and copolymers
5. Learn about different methods of finding out average molecular weight of polymers
6. Differentiate between glass transition temperature (Tg) and crystalline melting point (Tm)
7. Determine of Tg and Tm
8. Know about solid and solution properties of polymers
9. 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.

(4 Lectures)

Functionality and its importance:

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bifunctional systems, Poly-functional systems.

(8 Lectures)

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.

(8Lectures)

Unit 3:

Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg). **(8 Lectures)**

Crystallization and crystallinity: Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point. **(4 Lectures)**

Nature and structure of polymers-Structure Property relationships. **(2 Lectures)**

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. **(8 Lectures)**

Polymer Solution: Criteria for polymer solubility and Solubility parameter. Thermodynamics of polymer solutions, entropy, enthalpy and free energy change of mixing of polymers solutions.
(4 Lectures)

Polymer Degradation- Thermal, oxidative, hydrolytic and photodegradation
(4 Lectures)

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, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].
(10 Lectures)

Practical:

CHEMISTRY PRACTICAL - DSE 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-Gravimetery-Differential Thermal analaysis) of polymers

Suggested Additional Experiment:

1. Purification of Monomer.
2. Emulsion Polymerization of a monomer.

References:

Theory:

- Seymour's Polymer Chemistry, Marcel Dekker, Inc.
- G. Odian: Principles of Polymerization, John Wiley.
- F.W. Billmeyer: Text Book of Polymer Science, John Wiley.
- P. Ghosh: Polymer Science & Technology, Tata Mcgraw-Hill.
- R.W. Lenz: Organic Chemistry of Synthetic High Polymers.
- S. M. Ashraf, S. Ahmad, U. Riaz, A Laboratory Manual of Polymers, I.K. International Publishing House (2008).

Practical:

• Malcohm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
• Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
• Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
• Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
• Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
• L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)
• Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)

- Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

Teaching Learning Process:

Chalk and Talk method, ICT enabled teaching. Students need to make presentations.

Assessment Methods:

Assessment through continuous evaluation, assignments, class tests, presentations, quiz, projects.

Keywords:

Bonding, texture, polymerization, degradation, polymer solution, crystallization, Properties, applications.

Research Methodology for Chemistry

Chemistry DSE2-4 (v)

Total Credits: 06 **(Credits: Theory-04, Practicals-02)**
(Total Lectures: Theory-75, Tutorial-1)

Objectives:

The objective of this paper is to formulate the research problems and connect the research outcomes to the society. 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-

1) Able to identify research problems.
2) Able to find out local solution.
3) Able to communicate the research at appropriate level.

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.**

(**20 Lectures)**

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.

(**20 Lectures)**

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 – 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. **Hazardous Chemicals in Households.**

(**12 Lectures)**

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**

(**13 Lectures)**

Exposure of chemistry softwares:

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

(**10 Lectures)**

References

Theory:

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. *Practical skills in chemistry 2nd Ed*. Prentice-Hall, Harlow, 2011.
- Hibbert, D. B. & Gooding, J. J.*Data analysis for chemistry*. Oxford University Press. 2006.
- Topping, J. *Errors of observation and their treatment. Fourth Ed*. Chapman Hall, London. 1984.
- Harris, D. C. *Quantitative chemical analysis. 6th Ed*., Freeman Chapters 3-5, 2007.
- Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis. Cambridge Univ, 2001.
- Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
- OSU safety manual 1.01.

Additional Resources:

- Introductory Biostatistics by Chap T Le.

Teaching Learning Process

- Lecture with conventional teaching aids, presentations, invited talks on thrusting areas, group discussions

Assessment Methods

- writing review on identified research problem
- Poster presentation
- university examination

75 % University Exam and 25 % Internal Assessment(Assigment, regularity and presentation)

Green Chemistry

Chemistry DSE 2-4(vi)
Total Credits: 06 **(Credits: Theory-04, Practicals-02)**
(Total Lectures: Theory-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 depleting, heaps and heaps of landfill s 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 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 learn the following

1. Understand the twelve principles of green chemistry and will build the basicunderstanding 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 willunderstand 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 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. Successstories 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

(5 Lectures)

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:

- Designing a Green Synthesis using these principles; Prevention of Waste/ by products; maximum incorporation of the materials used in the process into the final products , Environmental impact factor
- 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 ; waste or pollution prevention hierarchy
- Designing safer chemicals with minimum toxicity yet has the ability to perform the desired functions
- Green solvents: super critical fluids, 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
- 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, bio catalysis, asymmetric catalysis and photo catalysis.
- Design for degradation: A product should not persist after the commercial function is over e.g. soaps and detergents and some more
- 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 o carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.

(25 Lectures)

Unit 3:

Examples of Green Synthesis/ Reactions

- Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)
- Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction
- Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)

(10 Lectures)

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 (poly lactic 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.

(10 Lectures)

Unit 5:

Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimcry and green chemistry, biomimetic, multifunctional reagents , combinatorial green chemistry, mechanochemical and solventfree synthesis of inorganic complexes; co crystal controlled solid state synthesis (C^2S^3); Green chemistry in sustainable development.

(10 Lectures)

Practical:

(Credits: 2, Lectures: 60)

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

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

2. Using renewable resources
Preparation and characterization of biodiesel from vegetable oil preferably waste cooking oil.

3. Use of enzymes as catalysts
Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.

1. **Alternative Green solvents**

- Extraction of D-limonene from orange peel using liquid CO_2 prepared form dry ice.
- 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).

2. **Alternative sources of energy**

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

3. Reducing waste

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

References:

Theory:

- P.T. Anastas & J. C. Warner, Green Chemistry, Theory and Practice, Oxford University Press (1998).
- M. Lancaster , Green Chemistry An Introductory Text. RSC Publishing, 2nd Edition. ISBN: 978-1-84755-873-2 (2016).
- M. C. Cann & M. E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
- M. C. Cann and ,Thomas P Umile, Real world cases in Green chemistry vol 11, American chemical Society,Washington (2008)
- A.S. Matlack, Introduction to Green Chemistry, Marcel Dekker (2001).
- V. K. Alhuwalia and M.R. Kidwai,New Trends in Green chemistry, Anamalaya Publishers (2005)
- A. L Garay, A. Pichon and S.L. James, Chem Soc Rev, 36,846-855 (2007).
- http// Biomimicry.org/askingnature
- Janine Benyus: Innovations Inspired by nature,Harper collins 1997.

Practical:

- Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
- Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. *Green Chemistry Experiments: A monograph I.K. International Publishing House Pvt Ltd. New Delhi*, Bangalore ISBN978-93-81141-55-7 (2013).
- Pavia,D.L. Lamponam, G.H.& Kriz, G.S.W B Introduction to organic Laboratory Technique-A Microscale approach,4th Ed, Brrooks-Cole Laboratory Series for Organic chemistry,2006
- 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

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,12 principles of green chemistry,atom economy,waste minimization,green metric,green solvents,solvent free,catalyst,bio-catalyst,renewable energy sources,hazardous,renewable feedstock,ionic liquids,supercritical fluids,inherent safer design, green synthesis, co-crystal controlled solid state synthesis,sustainable development,Presidential green chemistry awards

---

Industrial Chemicals and Environment

(Chemistry DSE 2-4(vii)) **Total Credits: 06**
(Credits: Theory-04, Practicals-02)
(Total Lectures: Theory-60)

Objectives:

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

- 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:

1. What are the different toxic gases and their toxicity hazards.
2. Safe design systems for large scale production of industrial gases.
3. How Inorganic chemicals are manufactured, handled, stored.
4. Hazardous effects of the Inorganic Chemicals on human beings and vegetation.
5. Why Ultra-Pure metals are required for the semiconducting technologies.
6. Composition of air, various Air Pollutants, Control measures of Air Pollutants.
7. Effects of Air Pollutants: Global Warming, Ozone Depletion
8. Different Sources of Water, Water quality parameters, Impacts of Water Pollution.
9. Water treatment and purification methods.
10. Different industrial effluents and their treatment methods.
11. Different Sources of Energy.
12. How nuclear waste is generated and its disposal?
    Study of nuclear disasters.
13. What is Green Chemistry and its importance in Chemical Industries?
    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.

(6 Lectures)

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

(10 Lectures)

Unit 3:

Industrial Metallurgy: Preparation of ultrapure metals for semiconductor technology.

(4 Lectures)

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).

(15 Lectures)

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 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.

(15 Lectures)

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.

(10 Lectures)

References:

- K.H. Buchel, H.H.Moretto, P.Woditsch, Industrial Inorganic Chemistry , Wiley-VCH, Second Edition (2003)
- E. Stocchi:Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
- R.M. Felder, R.W. Rousseau:Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
- J. A. Kent: Riegel'sHandbook of Industrial Chemistry, CBS Publishers, New Delhi.
- S. S. Dara:A Textbook of Engineering Chemistry, S. Chand & Company Ltd. New Delhi.
- A. K. De, Environmental Chemistry: New Age International Pvt., Ltd, New Delhi, , Eight Edition(2017)
- S. M. Khopkar,Environmental Pollution Analysis: Wiley Eastern Ltd, New Delhi.
- S.E. Manahan, Environmental Chemistry, CRC Press (2005).
- G.T. Miller, Environmental Science 11th edition. Brooks/ Cole (2006).

Practical:
(Credits: 2, Lectures: 60)

CHEMISTRY PRACTICAL-DSE 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:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
- R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
- J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
- S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
- A.K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
- S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.

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, Debate.
- To get recent information through the internet.

Assessment Methods:

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

Keywords:

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

---

Instrumental Methods of Chemical Analysis

(Chemistry DSE 2-4(viii) **Total Credits: 06**
(Credits: Theory-04, Practicals-02)
(Total Lecture: Theory- 60)

Objectives:

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

2. Knowledge of analytical data analysis and classification of analytical methods.
3. Basic components in Infrared , UV, Visible and near IR and Mass spectrophotometer.
4. Advantages of Fourier-Transform Infrared (FTIR) and NMRspectroscopy.
5. Portable instrumentation and issues regarding quality assurance and quality control.
6. Single and Double Beam instruments
7. Interpretation like quantification, mixtures, absorption vs. fluorescence and the use of time, photoaccoustic, fluorescent tags.
8. Separation techniques like Chromatography, Electrophoresis and DNA techniques
9. Elemental analysis,
10. Electroanalytical Methods, Radiochemical Methods , X-ray analysis and electron spectroscopy.

Learning Outcomes:

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

- How to handle Analytical data.
- Basic Components of IR , FTIR , UV-Visible and Mass spectrometer.
- Interpretation of IR, FTIR, UV-visible spectra and their applications.
- Signal detections in photocells, photomultipliers, etc.
- Use of single and double beam instruments.
- Separations techniques like Chromatography, DNA techniques.
- Mass spectra and its applications.
- Elemental analysis, NMR spectroscopy, Electroanalytical Methods, Radiochemical Methods , X-ray analysis and electron spectroscopy.

Unit 1:

Introduction to analytical methods of data analysis:

Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiations.

(**4 Lectures**)

Unit 2:

Molecular spectroscopy:

Infrared spectroscopy: Interaction of radiations with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier-Transform Infrared (FTIR) spectroscopy.

Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.

(8 Lectures)

Unit 3:

UV-Visible/ Near IR Spectroscopy

Emission, absorption, fluorescence and photoaccoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, placement of sample relative to dispersion, resolution), Detection of signal (photocells, photomultipliers, diode arrays, sensitivity and S/N), Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoaccoustic, fluorescent tags).

(8 Lectures)

Unit 4:

Separation techniques

Chromatography: Gas chromatography, liquid chromatography, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Detection: simple vs. specific (gas and liquid), Detection as a means of further analysis (use of tags and coupling to IR and MS), Electrophoresis (plates and capillary) and use with DNA analysis. *Immunoassays and DNA techniques.*

(8 Lectures)

Unit 5:

Mass spectroscopy:

Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, detection and interpretation.

(8 Lectures)

Unit 6:

Elemental analysis:

Mass spectrometry (electrical discharges).
Atomic spectroscopy**:** Atomic absorption, Atomic emission, and Atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wave length separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

(8 Lectures)

NMR spectroscopy:Principle,Instrumentation,Factors affecting chemical shift,Spin-coupling, Applications.

(4 Lectures)

Electroanalytical Methods: Potentiometry & Voltammetry.

(4 Lectures)

Radiochemical Methods.

(4 Lectures)

X-ray analysis and electron spectroscopy (surface analysis)

(4 Lectures)

References:

- Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
- Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.
- P.W. Atkins: Physical Chemistry.
- G.W. Castellan: Physical Chemistry.
- C.N. Banwell: Fundamentals of Molecular Spectroscopy.
- Brian Smith: Infrared Spectral Interpretations: A Systematic Approach.

- W.J. Moore: Physical Chemistry.

Practical:
(Credits: 2, Lectures: 60)

DSE LAB: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS

1. Determination of the isoelectric pH of a protein.
2. Titration curve of an amino acid.
3. Determination of the void volume of a gel filtration column.
4. Determination of a Mixture of Cobalt and Nickel (UV-visible spectroscopy).
5. Study of Electronic Transitions in Organic Molecules (i.e., acetone in water).
6. IR Absorption Spectra (Study of Aldehydes and Ketones).
7. Determination of Calcium, Iron, and Copper in Food by Atomic Absorptionspectroscopy.
8. Quantitative Analysis of Mixtures by Gas Chromatography (i.e., chloroform and carbon tetrachloride).
9. Separation of Carbohydrates by HPLC.
10. Determination of Caffeine in Beverages by HPLC.
11. Potentiometric Titration of a Chloride-Iodide Mixture.
12. Cyclic Voltammetry of the Ferrocyanide/Ferricyanide Couple.
13. Use of Nuclear Magnetic Resonance instrument and to analyse the spectra of methanol and ethanol
14. Use of fluorescence to do “presumptive tests” to identify blood or other body fluids.
15. Use of “presumptive tests” for anthrax or cocaine.
16. Collection, preservation, and control of blood evidence being used for DNA testing.
17. Use of capillary electrophoresis with laser fluorescence detection for nuclear DNA (Y chromosome only or multiple chromosome).
18. Use of sequencing for the analysis of mitochondrial DNA.
19. Laboratory analysis to confirm anthrax or cocaine.
20. Detection in the field and confirmation in the laboratory of flammable accelerants or explosives.
21. Detection of illegal drugs or steroids in athletes.
22. Detection of pollutants or illegal dumping.
23. Fibre analysis.

At least 10 experiments to be performed.

Reference:

Please add references

Teaching Learning Process:

- Conventional chalk and board teaching,
- Class interactions and group discussions
- Power point presentation on important topics.

Assessment Methods:

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

Keywords:

Analytical methods of data analysis, Infrared spectroscopy, UV-Visible spectroscopy, Chromatographic Techniques,Mass spectra,Elemental analysis methods, NMR spectroscopy, Electroanalytical methods, Radiochemical methods, X-ray analysis, Electron spectroscopy

SKILL-ENHANCEMENT COURSES (SEC)

IT SKILLS FOR CHEMISTS

ChemistrySEC1-4(i) **Total Credits: 04**
(Credits: Theory-02, Practicals-02)
(Hands on Exercises: 60 Lectures)

Objectives:

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

Course Learning Outcomes:

After completing this course, a student is expected to:

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

Unit 1:

Mathematics

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

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.
Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).
Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms).Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).
Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

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

Unit 2:

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

Unit 3:

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

Unit 4:

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

Unit 5:

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

Practical:

The major emphasis of the course is on hands on learning that will be carried out during practical class.

References:

- McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
- Mortimer, R. Mathematics for Physical Chemistry. 3 Ed. Elsevier (2005).
- Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- Yates, P. Chemical calculations. 2 Ed. CRC Press (2007).
- Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001).
- Noggle, J. H. Physical chemistry on a Microcomputer. Little Brown & Co. (1985).
- Venit, S.M. Programming in BASIC: Problem solving with structure and style. Jaico Publishing House: Delhi (1996).

Teaching Learning Process:

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

Assessment Methods:

Assessment on solving chemistry related problems using spreadsheet.
Presentation on documentation preparation on any chemistry topic involving tables and graphs.
Semester end practical and theory examination.

Keywords:

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

---

BASIC ANALYTICAL CHEMISTRY

ChemistrySEC1-4(ii) **Total Credits: 04**
(Credits: Theory-02, Practicals-02)
(Hands on Exercises: 60 Lectures)

Objectives:

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

Knowledge of chemical analysis including water and soil, separation techniques like Chromatography, Column, ion-exchange chromatography, etc. Instrumental demonstrations of flame photometry and determinations of macro-nutrients using flame photometry.

Learning Outcomes:

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

1. How to handle analytical data
2. How to determine composition and pH of soil which can be useful in agriculture
3. Quantitative analysis metal ions in water
4. Separations techniques
5. Estimation of macro nutrients using Flame photometry

Unit 1:

Introduction:

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

(4 Lectures)

Unit 2:

Analysis of soil:

Composition of soil, Concept of pH and its measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators

a. Determination of pH of soil samples.

b. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

(12 Lectures)

Unit 3:

Analysis of water:

Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.
a. Determination of pH, acidity and alkalinity of a water sample.
b. Determination of dissolved oxygen (DO) of a water sample.

(12 Lectures)

Unit 4:

Chromatography:

Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.
Paper chromatographic separation of mixture of metal ion (Ni^{2+} and Co^{2+}).

(12 Lectures)

Unit 5:

Ion-exchange:

Column, ion-exchange chromatography etc.

Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Suggested Applications (Any one):
a. To study the use of phenolphthalein in trap cases.
b. To analyze arson accelerants.
c. To carry out analysis of gasoline.

(10 Lectures)

Unit 6:

Instrumental demonstrations:

a. Estimation of macro-nutrients: Potassium, Calcium, Magnesium in soil samples by flame photometry.
b. Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.
c. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in soft drink.

(10 Lectures)

References:

- Willard, H. H. *Instrumental Methods of Analysis*, CBS Publishers, 1988.
- Skoog, D.A. and Leary, J.J., *Instrumental Methods of Analysis*, Saunders College Publications, New York, 1992
- Skoog, D.A.; West, D.M. and Holler, F.J. *Fundamentals of Analytical Chemistry 6th Ed.,* Saunders College Publishing, Fort Worth, 1992
- Harris, D. C. *Quantitative Chemical Analysis 7th Ed.*, W. H. Freeman and Co., New York, 2007
- Dean, J. A. *Analytical Chemistry Handbook*, McGraw Hill, 2007
- Day, R. A. and Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India, 1991.
- Freifelder, D. *Physical Biochemistry 2nd Ed.,* W.H. Freeman and Co., N.Y. 1982
- Cooper, T.G. (Ed.) *The Tools of Biochemistry,* John Wiley and Sons, N.Y. 1977
- Svehl a, G. , *Vogel's Qualitative Inorganic Analysis 7th Ed*., Prentice Hall, 1996
- Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M.J.K., *Vogel's Quantitative Chemical Analysis 6th Ed.,* Prentice Hall, 2007.
- Robinson, J.W. *Undergraduate Instrumental Analysis 5th Ed.,* Marcel Dekker, Inc., New York, 1995
- Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.

Teaching Learning Process:

- Conventional chalk and board teaching,
- Class room interactions and group discussions
- Lab demonstrations and experiments after completion of theory part
- ICT enabled classes

Assessment Methods:

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

Keywords:

Analytical chemistry, sampling, accuracy, precision, significant figures, Soil analysis, Analysis of water, Chromatography, Ion exchange chromatography, Flame photometry

---

CHEMICAL TECHNOLOGY AND SOCIETY

ChemistrySEC1-4(iii) **Total Credits: 04**
(Credits: Theory-02, Practicals-02)
(Hands on Exercises: 60 Lectures)

Objectives:

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

Course Learning Outcomes:

The students will be able to learn:

- Use of basic chemistry to chemical engineering
- Various chemical technology used in industries
- To develop scientific solutions for societal needs

Unit 1:

Chemical Technology

Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical

technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Society

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

Sources of energy

Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar, Hydrogen, geothermal, Tidal and Hydel

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

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

Natural Polymers

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

Basics of drug synthesis

Application of genetic engineering.

Teaching Learning Process:

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

Assessment Methods:

- Internal assessment of 25% marks including class attendance.
- Theory paper of 75% marks

Keywords:

Chemical Technology; Society; Energy; Polymer; Pollutants

CHEMINFORMATICS

CHEMISTRY SEC 1-4 (iv)

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

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

Objectives:

The aim of the course is to introduce the students to computation 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:

The student will be able to learn:

1. 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
2. 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,

(2 Lectures)

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.

(2 Lectures)

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.

(6 Lectures)

Unit 4:

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

(6 Lectures)

Unit 5:

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

(6 Lectures)

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.

(8 Lectures)

Practical:

Practicals/Hands on Exercises: (4 Periods per week / 60 Periods)

1. Overview of Rational Drug Design, Ligands and Targets

2. In silico representation of chemical information

- CIF IUCr Crystallographic Information Framework
- CML Chemical Markup Language
- SMILES -- Simplified Molecular Input Line Entry Specification
- InChi -- IUPAC International Chemical Identifier
- 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:

•Andrew R. Leach & Valerie, J. Gillet (2007) An introduction to Chemoinformatics.Springer: The Netherlands.
•Gasteiger, J. & Engel, T. (2003) Chemoinformatics: A text-book. Wiley-VCH
•Gupta, S. P. (2011) QSAR & Molecular Modeling. Anamaya Pub.: New Delhi.
Gasteiger, J. Handbook of cheminformatics: from data to knowledge in 4 volumes.

Additional Resources:

Bajorath, Jürgen (Ed.) 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:

BUSINESS SKILLS FOR CHEMISTS

CHEMISTRY SEC 1-4 (v)
Total Credits: 04 (Credits: Theory-02, Practicals-02)
(Total Lecture: Theory- 30, Practicals-60)

Objectives:

1. To enhance the Business and Entrepreneurial Skills of undergraduate chemistry students and improve their Employment Prospects.
2. To orient the students to understand the Industry linkage with Chemistry, Challenges and Business Opportunities.
3. To Introduce the concept of Intellectual Property Rights, Patents and Commercialisation of innovations.

Learning Outcomes:

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

1. Student will learn Basics of Business Concepts and Project Management Skills.
2. They will learn to understand the product development and Business Planning that includes Environmental Compliancy.
3. Through real life case studies, they will learn the process by which technical innovations are conceived and converted into successful business ventures.
4. The course also orients the students on the Intellectual Property Rights and Patents to drive business viability and Commercialisation of Innovation.
5. After going through this course the students will be able to 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

(10 Lectures)

Unit 2:

Business Basics

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

(12 Lectures)

Unit 3:

Project Management

Different stages of a project

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

(10 Lectures)

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

(10 Lectures)

Unit 5:

Intellectual Property Rights

- Introduction to IPR & Patents

(6 Lectures)

Unit 6:

Environmental Hazards

Industries involving Hazardous chemicals. Importance of development of cost-effective alternative technology. Environmental Ethics.

(12 Lectures)

Practical:

- 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:

- www.rsc.org
- Lawerence I. Nwaeke, Business Concepts and Perspectives
- Titus De Silva, Essential Management Skills for Pharmacy and Business Managers

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

---

INTELLECTUAL PROPERTY RIGHTS

CHEMISTRY SEC 1-4 (vi)
Total Credits: 04
(Total Lecture: Theory-60)

Objectives:

1. 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.
2. 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.
3. The course may also provide cursory understanding of the overall IP ecosystem in the country.

Learning Outcomes:

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

1. Learn theoretical concepts of evolution of Intellectual Property Laws, and to differentiate between the different kinds of IP.
2. Know the existing legal framework relating to IP in India.
3. 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.

(8 Lectures)

Unit 2:

Copyright and Related rights

Introduction to copyright and its relevance, Subject matter & conditions of protection, Ownership and term of copyright, Rights under copyright law, Infringement of copyright and remedies, Exceptions to infringement/ Public rights.

(10 Lectures)

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.

(15 Lectures)

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 registerability of trademark : Distictiveness & 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

(8Lectures)

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

(12 Lectures)

Unit 6:

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

(7Lectures)

Practical:

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

References:

- Neeraj Pandey and Khusdeep Dhami; Intellectual Property Rights, PHI Learning Pvt. Ltd.,India,2014
- N.K.Acharya; Text Book of Intellectual Property Rights,Asia Law House,2001.
- P.Ganguli, Intellectual Property Rights : unleasing the knowledge economy,Tata McGraw Hill,2001.

Additional Resources:

- https://www.wipo.int
- V.K.Ahuja; Law Relating to Intellectual Property Rights,Lexis Nexis,2017.
- B.L.Wadehra; Law Relating to Patents, Trade Marks, Copyright, Designs &Geographical Indications; Universal law Publishing Pvt. Ltd., India 2000.
- 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 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%. The students will earn 02 credits after completion/ passing of this course.

Keywords:

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

ANALYTICAL CLINICAL BIOCHEMISTRY

CHEMISTRY SEC 1-4 (vii)

Total Credits: 04 (Credits: Theory-02, Practicals-02)
(Total Lectures: Theory- 30, Practicals-30)

Objectives:

1. To deliver information about biochemically significant features of the proteins, enzymes, nucleic acids and lipids, using suitable examples. This includes classification, properties and biological importance of biomolecules.
2. To give an overview of drug receptor interaction and Structure Activity Relation (SAR) studies.
3. To introduce the concept of genetic code and concept of heredity.
4. Key emphasis is placed on understanding the basic principles that govern the biological functions of biomolecules .

Learning Outcomes:

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

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

Unit 1:

Metabolism

Biological importance of carbohydrates and proteins, Introduction to Metabolism (catabolism, anabolism), ATP: the universal currency of cellular energy, Outline of catabolic pathways of Fats, Proteins and Carbohydrate-Glycolysis, Alcoholic and Lactic acid Fermentation, Krebs Cycle.

(4 Lectures)

Unit 2:

Enzymes

Nomenclature,classification, Characterisation, Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, Specificity of enzyme action (Including stereospecifity), Enzyme inhibitors and their importance, Introduction to Biocatalysis: Importance in —Green Chemistry and Chemical Industry.Drug action-receptor theory. Structure – activity relationships of drug molecules, binding role of –OH group,-NH_2 group, double bond and aromatic ring.

(8 Lectures)

Unit 3:

Lipids

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

(6 Lectures)

Unit 4:

Nucleic Acids

Components of Nucleic acids: Adenine, guanine, thymine and Cytosine (Structure only), Other components of nucleic acids, Nucleosides and nucleotides (Numbering), Structure of DNA (Watson-Crick model) and RNA(types of RNA), Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation.

(6 Lectures)

Unit 5:

Biochemistry of disease

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

(6 Lectures)

Practical:

Chemistry SEC Lab: Analytical Clinical Biochemistry

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

References

Theory:

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. *Practical skills in chemistry 2nd Ed*. Prentice-Hall, Harlow, 2011.
- T.G. Cooper: Tool of Biochemistry.
- Keith Wilson and John Walker: Practical Chemistry.
- Alan H Gowenlock: Varley's Practical Clinical Biochemistry.

- Thomas M. Devlin: Textbook of Biochemistry.
- Berg, J. M., Tymoczko, J. L. &Stryer, L. Biochemistry 7th Ed., W. H. Freeman.
- U. Satyanarayana, U. Chakrapani. Biochemistry, 3rd Edition, Books and Allied (P) Ltd.
- Albert L. Lehninger, David L. Nelson, MichaelM. Cox, Princople of Biochemistry,7th Edition,Worth Publisher.
- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Introduction to practical biochemistry by S K Swahney and RandhirSingh ,Nerosa Publications

Teaching Learning Process:

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

Assessment Methods:

- Students evaluation will be 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.

GREEN METHODS IN CHEMISTRY

CHEMISTRY SEC 1-4 (viii)

Total Credits: 04 (Credits: Theory-02, Practicals-02)
(Total Lectures: Theory- 30, Practicals-30)

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.
- Students will acquire the knowledge of the twelve principles of Green Chemistry and how to apply in Green synthesis.
- Spread awareness about the benefits of using green chemistry.
- By studying the course students will have the idea of Biocatalytic Process—Conversion of Biomass into chemicals.
- To make the students as the policy maker in solving the major issues of the chemical industries and environmental issues.

Learning Outcomes:

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

- Get idea of Toxicology, environmental law, energy and the environment
- Aspiring students those who are hoping to pursue a career can take manufacturing jobs in pharmaceuticals, polymers or food engineering.
- Students can think to design and develops materials and processes that reduce the use and generation of hazardous substances in Industry.
- Students can think a chemical method for recovering metals from used electronics
- Students can get ideas of innovative approaches to environmental and societal challenges.
- 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 reformations in these protocols so that the environmental credentialssome of the real-world examples where green chemistry has been incorporated to improve.
- Students will get idea of role of catalysts in the conversion pathways and how to focus on the optimization of catalyst efficiency and on the design of heterogeneous catalyst.
- Idea of resources, chemical composition of Biomass, utilization of waste, green chemical technologies for their conversion to valuable chemicals.

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).

(8 Lectures)

Unit 2:

Twelve Principles of Green Chemistry

- A brief introduction of the twelve principles of the Green Chemistry with their explanations

- Designing a Green Synthesis using these Principles with emphasis on
    - *Prevention of Waste / Byproducts*
    - *Atom economy, 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 of carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.

(14 lectures)

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 (poly lactic acid) made from corn.

(8 Lectures)

Practical:

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 productsand 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:

- P. T. Anastas & J. C. Warner : Green Chemistry- Theory and Practice, Oxford University Press, (1998)
- Lancaster, Mike Green Chemistry: An Introductory Text: RSC Publishing, (2010) 2nd Edition, ISBN 978-1-84755-873-2.
- A.S. Matlack : Introduction to Green Chemistry, Marcel Dekker (2001)
- M. C. Cann & M. E. Connely : Real-World Cases in Green Chemistry, American Chemical Society, Washington, (2000)
- M. C. Cann and Thomas P. Umile ; Real-World Cases in Green Chemistry, American Chemical Society.
- Ryan, M.A. Introduction to Green Chemistry, Tinnesand; (Ed), American Chemical Society, Washington DC (2002)

Practical:

- Kirchof, M. & Ryan, M. A. Greener approaches to undergraduate chemistry experiment. American Chemical Society, Washington DC (2002).
- Sharma, R. K.; Sidhwani, I. T. & Chaudhari, M.K. Green Chemistry Experiments: A monograph I.K. International Publishing House Pvt. Ltd. New Delhi, Bangalore ISBN 978-93-81141-55-7 (2013).
- Pavia, D. L., Lampman, G. H. & Kriz, G. S.; Introduction to organic laboratory technique: A contemporaray approach. W.D Saunders Publication Philadalphia 1976.
- Sharma R. K., Sharma, C., & Sidhwani, I.T. (2010). Solventless and one-pot synthesis of Cu(II) phthalocyanine complex: a green chemistry experiment. Journal of Chemical Education, 2010, 88(1), 86-88.
- 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.
- 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:

- Power point presentations.
- Discussions on the problems
- Asking students to make charts showing the solutions of the surrounding problems
- Real world problems solutions discussion
- quiz
- Test
- Assignments

Keywords:

Green Chemistry, 12 Principles

PHARMACEUTICAL CHEMISTRY

CHEMISTRY SEC 1-4 (ix)

Total Credits: 04 (Credits: Theory-02, Practicals-02)
(Total Lecture: Theory- 30, Practicals-30)

Objectives:

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

Learning Outcomes:

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

1. Students will gain insight into retro-synthesis approach in relation to drug design and drug discovery.
2. The students will learn synthesis of major drug classes.
3. The students will be able to understand the fermentation process and production of ethanol, citric acids, antibiotics and some classes of vitamins

Unit 1:

Introduction

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

(7 Lectures)

Unit 2:

Drugs and Pharmaceuticals

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

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

Unit 3:

Fermentation

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

8 Lectures

Practical:

Chemistry SEC Lab: Pharmaceutical Chemistry

1. Preparation of Aspirin and its analysis.
2. Preparation of paracetamol and its analysis.
3. Preparation of sulphacetamide or sulpdonamide and its analysis.
4. Determination of alcohol contents in liquid durgs/galenicals.
5. Determination of ascorbic acid in Vitamin C tablets by iodometric or coulometric titrations.
6. Synthesis of Ibuprofen.
7. Analysis of commercial vitamin C tablets by iodometric and coulometric titrimetry

References:

- Patrick: Introduction to Medicinal Chemistry, Oxford University Press, UK.
- Hakishan, V.K. Kapoor: Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan, Pitampura, New Delhi.
- William O. Foye, Thomas L., Lemke , David A. William: Principles of Medicinal Chemistry, B.I. Waverly Pvt. Ltd. New Delhi.

- Synthesis of Ibuprofen. in the Introductory Organic Laboratory Source: Richard A. Kjonaas*, Peggy E. Williams, David A. Counce, and Lindsey R. Crawley,Department of Chemistry and Physics, Indiana State University, Terre Haute, Indiana 47809, United States. J. Chem. Educ., 2011, 88 (6), pp 825–828 DOI: 10.1021/ed100892p.
- Analysis of commercial vitamin C tablets by iodometric and coulometric titrimetry Source: Daniel G. Marsh, Deborah L. Jacobs, and Hans Veening J. Chem. Educ., 1973, 50 (9), p 626. DOI: 10.1021/ed050p626

Teaching Learning Process:

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

Assessment Methods:

Students evaluation done on the basis of regular class tests, presentations and assignments during the course as per the curriculum.

Keywords:

Retro-synthesis , drug discovery, design and synthesis, side effects, Fermentation.

CHEMISTRY OF COSMETICS AND PERFUMES

CHEMISTRY SEC 1-4 (x)

Total Credits: 04 (Credits: Theory-02, Practicals-02)
(Total Lectures: Theory-30, Practical-60)

Objectives:

Cosmetic plays an important role in our everyday lives as they make an individual's appearance more attractive and boost one's self-esteem and confidence. Keeping in view the tremendous potential which the cosmetic industry has today around the globe, this course will be useful for introducing someone to the world of cosmetic chemistry. This has been designed to impart the theoretical and practical knowledge on basic principles of cosmetic chemistry, manufacture, formulation of various cosmetic products

Learning outcomes:

Students will be able to learn:

1. Basic of cosmetics, various cosmetic formulation, ingredients and their roles in cosmetic products.
2. Use of safe, economic and body-friendly cosmetics
3. To prepare new innovative formulations

Unit 1:

Cosmetics- Definition,, History, Classification, Ingredients, Nomenclature, regulations

(4 Lectures)

Unit 2:

Face Preparation: Structure of skin, Face powder, Compact powder, Talcum powder

(6Lectures)

Unit 3:

Skin Preparation: Face cream, vanishing cream, cold cream, suntan cream, lather shaving cream

(5Lectures)

Unit 4:

Hair preparation: Structure of hair, classification of hair, Hair dye- classification – temporary, semi-permanent, demi permanent, permanent, formulation, hair sprays, shampoo- types of shampoo, conditioners

(6Lectures)

Unit 5:

Colored preparation: Nail preparation Structure of nail, Nail lacquers, Nail polish remover Lipsticks

(4 Lectures)

Unit 6:

Personal Hygiene products: Antiperspirants and Deodorants, Oral hygiene products, Flavours and Essential oils

(6Lectures)

Practical:

Practicals/ Hands on session (4 periods /week)

1.Preparation of talcum powder.
2.Preparation of shampoo.
3.Preparation of enamels.
4.Preparation of face cream.

5.Preparation of nail polish and nail polish remover.

6. Preparation of hand Wash
7. Preparation of hand sanitizer
8. Preparation of body lotion
9. Preparation of soap
10. Preparation of tooth powder
11. Preparation of tooth paste

References:

- Textbook of Cosmetics; M Vimaladevi; CBS Publishers & Distributors; 2015, ISBN 81-239-1103-3
- Handbook of Cosmetic Science and Technology; Edited by Andre´ O. Barel, Marc Paye, Howard I. Maibach; Informa Healthcare;2009, ISBN 978-1-4200-6963-1
- Text Book of Cosmetics; Dr Akanksha Garud, Dr PK Sharma, Dr Navneet Garud; Pragati Prakashan; 2012, ISBN 978-93-5006-691-1
- Pharmaceutics and Cosmetics; Praveen K. Gupta,Sanjeev K. Gupta; Pragati Prakashan;2011 ISBN 978-81-8398-995-4
- Poucher's perfumes , Cosmetic and Soap, H.Butler, springer netherlands, 2000, ISBN 0751404799
- Chemistry of Cosmetics; R. Kumari; Prestige Publisher, 2018, ISBN 978-81-936512-3-0

Additional Resources:

- COSMETIC AND TOILETRY FORMULATIONS; Ernest W. Flick, Noyes Publications / William Andrew Publishing, ISBN: 0-8155-1454-9
- Natural Ingredients for Cosmetics; EU Survey 2005
- FORMULATION GUIDE FOR COSMETICS; The Nisshin OilliO Group, Ltd.
- Functional Ingredients & Formulated Products for Cosmetics & Pharmaceuticals; NOF Corporation

Teaching Learning Process:

- Conventional chalk and board teaching with power point presentation, you tube videos. and presentations from students on relevant topics.
- Theory coupled with preparation of cosmetic products in lab.

Assessment Methods:

As per Delhi University rule.

Keywords:

Cosmetic Products, Ingredients, Formulations, Raw materials, Lab. preparation, Ideal characteristics

PESTICIDE CHEMISTRY

CHEMISTRY SEC 1-4 (xi)
Total Credits: 04 (Credits: Theory-02, Practicals-02)
(Total Lectures: Theory- 30, Practicals-30)

Objectives:

Pesticide play 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 to prevention of certain diseases, which conserves health and has saved the lives of millions of people and domestic animals.

Learning Outcomes:

Students will 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:

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).

Unit 2:

Botanical insecticides [Nostructure elucidation or synthesis is required for the following compounds:]
Alkaloids (Nicotine); Pyrethrum (natural and synthetic pyrethroids); Azadirachtin; Rotenone and Limomnen

Unit 3:

Pesticide formulations (Wettable powders, Surfactants, Emulsifiable concentrates, Aerosols, Dust and Granules)

Practical:

1. To carryout market survey of potent pesticides with details as follows:
a) Name of pesticide b) Chemical name, class and structure of herbicide 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. Preparation of simple Organochlorine pesticides.
3.To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
4. To calculate active ingredient in given sample of pesticide formulations as per BIS specifications.

References:

- Perry, A.S., Yamamoto, I., I. Shaaya and R. Perry, Insecticides in Agriculture and Environment, Narora Publishing House.
- R.J. Kuhr, H.W. Derough, Carbamate Insecticides, Chemistry, Biochemistry and Toxicology, CRC Press.

Teaching Learning Process:

Chalkboard education is best for teaching theory topics.

Assessment Methods:

No Change Required

Keywords:

Structure Activity Relationship (SAR), Organochlorines, Organophosphates, Carbamates, Quinones, Anilides, Botanical, Alkaloids, Pyrethrum, Azadirachtin, Rotenone, Limomnen, Pesticide formulations

FUEL CHEMISTRY

CHEMISTRY SEC 1-4 (xii)
Total Credits: 04 **(Credits: Theory-02, Practicals-02)**
(Total Lectures: Theory- 30, Practicals-30)

(Total Lecture: 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.

Unit 2:

Coal: 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.

Unit 3:

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

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.

Unit 5:

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

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 their determination.

Practical:

- Test Methods for Petroleum products
- To prepare biodiesel from vegetable oil
- Calorific value of a fuel
- Characterization of different petroleum products using UV and IR

References:

Industrial Chemistry, Vol -I, Ellis Horwood Ltd. UK.

Teaching Learning Process:

- Lectures by regular Faculty
- 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.

Keywords:

Energy; Fuels; Petroleum; Biofuels; Synthetic

GENERIC ELECTIVE

Atomic Structure, Bonding, General Organic
(ChemistryGE i)

CHEMISTRY GE- I

Total Credits: 06 **(Credits: Theory-04, Practicals-02)**
(Total Lecture: Theory- 60, Practicals-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-

1. 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.
2. Able to draw the plausible structures and geometries of molecules using Radius Ratio Rules, VSEPR theory and MO diagrams (homo- & hetero-nuclear diatomic molecules).
3. Understand and explain the differential behavior of organic compounds based on fundamental concepts learnt.
4. Formulate the mechanism of organic reactions by recalling and correlating the fundamental properties of the reactants involved.
5. Learn and identify many organic reaction mechanisms including Free Radical Substitution, Electrophilic Addition and Electrophilic Aromatic Substitution.

Unit 1

Section A: Inorganic Chemistry-1 (30 Periods)

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 wavefunctions (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, 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 1^{st} and 2^{nd} periods (including idea of *s-p* mixing) and heteronuclear diatomic molecules such as CO, NO and NO^+.

(Lectures:16)

Section B: Organic Chemistry-1

Unit 3 Fundamentals of Organic Chemistry

Electronic Displacements: Inductive Effect, ElectromericEffect, Resonance, Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis. and Reaction intermediates: Carbocations, Carbanions and free radicals. Electrophiles and nucleophiles Aromaticity: Benzenoids and Hückel's rule.

(Lectures :8)

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. $KMnO_4$) andtrans-addition (bromine), Addition of HX (Markownikoff'sand 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:

Section A: Inorganic Chemistry - Volumetric Analysis

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid 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. Detection of extra elements (N, S, Cl, Br, I) in organic compounds
4. Separation of mixtures by Chromatography: Measure the R_f value in each case (combination of two compounds to be given)

(a) Identify and separate the components of a given mixture of 2 amino acids (glycine,aspartic acid, glutamic acid, tyrosine or any other amino acid) by radial/ascending paper chromatography

(b) Identify and separate the sugars present in the given mixture by radial/ascending paper chromatography.

References:

Theory:

- J. D. Lee: *A new Concise Inorganic Chemistry,* E L. B. S.17
- F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry,* John Wiley.
- Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry,* John Wiley.
- James E. Huheey, *Ellen Keiter and Richard Keiter: Inorganic Chemistry: Principles of Structure and Reactivity,* Pearson Publication.
- T. W. Graham Solomon: *Organic Chemistry, John Wiley and Sons.*
- Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry,* Orient Longman.
- E. L. Eliel: *Stereochemistry of Carbon Compounds,* Tata McGraw Hill.
- I. L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
- R. T. Morrison & R. N. Boyd: *Organic Chemistry,* Prentice Hall.
- Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry,* S. Chand
- Atkins, Overton, Rourke, Weller, Armstrong, Shriver and Atkins *Inorganic Chemistry,* Oxford

Practical:

- Vogel's Qualitative Inorganic Analysis, A.I. Vogel, Prentice Hall, 7th Edition.
- Vogel's Quantitative Chemical Analysis, A.I. Vogel, Prentice Hall, 6th Edition.
- Textbook of Practical Organic Chemistry, A.I. Vogel , Prentice Hall, 5th Edition.
- Practical Organic Chemistry, F. G. Mann. & B. C. Saunders, Orient Longman, 1960.

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:

Following **assessment methods** can be adopted to evaluate the students:

- Conventional Class tests
- Open Book tests
- Assignments
- Online tests --objective or subjective
- Quizzes
- Presentation on a topic in front of the classmates
- Performing a new experiment based on the concepts learned in the course.

Keywords

Atomic structures, quantum numbers, lattice energy, stereochemistry, resonance, inductive effect, hyperconjugation

Chemical Energetics, Equillibria and Functional Organic Chemistry (Chemistry GE ii)

CHEMISTRY GE- II

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

Objectives:

The objective of this paper is to develop basic understanding of the chemical energetics, laws of thermodynamics, chemical and ionic equilibrium. To enable the students to understand the behaviour of electrolytes and their solutions. To acquaint students with the functional group approach to study organic compounds. To describe structure, methods of preparation and reactions for the following functional groups: Aromatic Hydrocarbons, Alkyl and Aryl Halides, Alcohols, Phenols and Ethers,aldehydes and ketones. To establish a relationship between the structure physical and chemical characteristic of compounds containing these functional groups.

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 for studying 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 outcome of a reaction
- Design newer synthetic routes for various organic compounds.

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.

(8 Lectures)

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.

(8 Lectures)

Unit 3:

Ionic Equilibria

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, 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. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

(12 Lectures)

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.

(5Lectures)

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 (SN1, SN2 and SNi),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 NaNH2/NH3 (Elimination-Addition Mechanism involving Benzyne Intermediate). Relative reactivity and strength of C-X bond in alkyl, allyl, benzyl, vinyl and aryl halides.

(11 Lectures)

Unit 6:

Alcohols, Phenols,Ethers,Aldehydes and Ketones

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 $KMnO_4$, acid $K_2Cr_2O_7$ 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, $NaHSO_3$, NH2-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-PondorffVerley reduction.

(14 Lectures)

Practical:

Section A: Physical Chemistry

Energetics:

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide. 3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts (KNO3, NH4Cl).
5. Determination of enthalpy of hydration of copper sulphate.

Ionic equilibria and pH measurements:

1. Measurement of pH of different solutions like aerated drinks, fruit juices, shampoos and soaps (use dilute solutions of soaps and shampoos to prevent damage to the glass electrode) using pH-meter.
2. Preparation of buffer solutions: (i)Sodium acetate-acetic acid (ii)Ammonium chloride-ammonium hydroxide 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)
Recrystallisation, determination of melting point and calculation of quantitative yields to be done.

1. Bromination of Phenol/Aniline
2. Benzoylation of amines/phenols
3. Oximeof aldehydes and ketones
4. 2,4-dinitrophenylhydrazoneof aldehydes and ketones
5. Semicarbazone of aldehydes and ketones

References:

Theory:

- W. Graham Solomons: Organic Chemistry, John Wiley and Sons.
- Peter Sykes: A Guide Book to Mechanism in Organic Chemistry, Orient Longman.
- I.L. Finar: Organic Chemistry (Vol. I & II), E. L. B. S.
- R. T. Morrison & R. N. Boyd: Organic Chemistry, Prentice Hall.
- Arun Bahl and B. S. Bahl: Advanced Organic Chemistry, S. Chand.
- G. M. Barrow: Physical Chemistry Tata McGraw Hill (2007).
- G. W. Castellan: Physical Chemistry 4th Edn. Narosa (2004).
- J. C. Kotz, P. M. Treichel& J. R. Townsend: General Chemistry Cengage Lening India Pvt. Ltd., New Delhi (2009).
- B. H. Mahan: University Chemistry 3rd Ed. Narosa (1998).
- R. H. Petrucci: General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985).

Practical:

- A.I. Vogel: Textbook of Practical Organic Chemistry, 5th edition, Prentice-Hall.
- F. G. Mann & B. C. Saunders, Practical Organic Chemistry, Orient Longman (1960).
- B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

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:

Students evaluation will be done on the basis of regular class test, assignments and presentations during the course.

Keywords:

Hydrocarbons, Haloalkanes and haloarenes, Alcohols, Phenols and Ethers,Aldehydes and Ketones

Solutions, Phase Equilibrium, Conductance, Electrochemistry and Functional Group Organic Chemistry-II (Chemistry GE iii)

CHEMISTRY GE- iii

Total Credits: 06 **(Credits: Theory-04, Practicals-02)**
(Total Lecture: Theory- 60, Practicals-60)

Objectives:

In Section A of this course students will learn about ideal and non-ideal solutions, Raoult's law, azeotropes, concept of EMF of a cell and measurement of emf of a cell. Nernst equation, Calculation of thermodynamic properties from EMF data. In Section B of this course, students will learn: Chemistry of carboxylic acids and their derivatives, Amines and diazonium salts,Active methylene compounds.The students will be introduced to the chemistry of Polynuclear hydrocarbons and heterocyclic compounds.

Learning Outcomes:

Students will be able to learn:

- Building on the concepts of functional group chemistry, this core course gives a better understanding of some other organic functional groups viz; carboxylic acids,theirderivatives,amines and diazonium salts.The chemistry of polynuclear hydrocarbons andheterocyclic compounds will be introduced in this course. The detailed reactions mechanistic pathways for relevant reactions will be discussed to unravel the spectrum of organic chemistry and the extent of organic transformations.

Section A: Physical Chemistry-2 (30 Lectures)

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. Distilllation 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.

(6 Lectures)

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, congurent and incongurent melting points (lead-silver, FeCl3-H2O and Na-K only).

(6 Lectures)

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).

(8 Lectures)

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-baser and oxidation-reduction only).

(10 Lectures)

Section B: Organic Chemistry-3 (30 Lectures)

Unit 5:

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

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.

Amines and Diazonium Salts Amines (aliphatic & aromatic)

Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction. Reactions: Hofmann vs Saytzeff elimination, carbylamine test, Hinsberg test, reaction 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.

(12 Lectures)

Unit 6:

Active methylene compounds

Preparation: Claisen ester condensation. Keto-enol tautomerism.

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

(6 Lectures)

Polynuclear and heteronuclear aromatic compounds:

Structure elucidation of naphthalene, preparation and properties of naphthalene and anthracene. Properties of the following compounds with reference to electrophilic and nucleophilic substitution: Furan, Pyrrole, Thiophene, and Pyridine. **(12 Lectures)**

Practical:

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 following potentiometric titrations: a) Strong acid vs strong base b) Weak acid vs strong base

Section B: Organic Chemistry

1. Systematic Qualitative organic analyses of organic compounds possessing monofunctional groups (Alcohols, Phenols, Carbonyl,-COOH)

References:

- G. M. Barrow: Physical Chemistry Tata McGraw Hill (2007).
- G. W. Castellan: Physical Chemistry 4th Ed. Narosa (2004).
- R. T. Morrison and R.N. Boyd; Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- I.L. Finar; Organic Chemistry (Vol 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Teaching Learning Process:

Conventional teaching methods as well as power point presentations. Group discussions.

Assessment Methods:

Student evaluation will be done on the basis of regular class test, assignments and presentations during the course.

Keywords:

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

Chemistry of s- and p-Block Elements, States of Matter and Chemical Kinetics
(Chemistry GE iv)

CHEMISTRY GE- iv

Total Credits: 06 (Credits: Theory-04, Practicals-02)
(Total Lecture: Theory- 60, Practicals-60)

Objectives:

The students will be able to:

Metallurgy

- To learn the fundamental principles of metallurgy.
- In a position to ascertain the method of extraction of a particular metal and also understands the importance of recovery of by-products during extraction.
- To gain an understanding of basic and practical applications in various fields of metals and alloy behavior and their manufacturing processes.

s- and p- block elements:

- This course illustrates the diversity and fascination of inorganic chemistry through the properties and utilities of s- and p-block elements in the periodic table.
- The course covers the systematic explanation of the various groups in order to learn the periodic trends in the properties of the elements.
- To understand the basic nature of each element as well as their diversity, and also understand how these feature affect the peculiar nature and function of the compounds.

Chemical Kinetics

- To define the average and instantaneous rate of reaction.
- To distinguish between elementary and complex reactions.
- To distinguish between order and molecularity.
- To derive integrated rate law equation for the first and second order reaction and determine the half-life of a reaction.
- To discuss the dependence of rate of reaction on pressure, concentration, temperature and catalyst.
- To discuss the general methods for determination of order of reaction
- To introduce concept of collision theory and activated complex theory.

States of Matter

Gases

- To discuss the postulates of kinetic theory of gases and derivation of kinetic gas equation.
- To discuss the deviation of real gas from ideal behaviour, compressibility factor, cause of deviation, van der Wallsequation state of real gases.
- To describe the conditions required for liquefaction of gases calculation from van der Walls equation
- To discuss Andrew's isotherm of CO2
- To describe the distribution laws of molecular velocities and energies (Maxwell Boltzmann distribution law).
- To explain most probable average and root mean square velocities and their temperature dependence
- To describe collision number, collision frequency and diameter
- To discuss the effect of temperature and pressure on the viscosity of gas.

Liquids

- To discuss the surface tension and viscosity of liquids and determination of surface tension by using Stalagmometer and coefficient of viscosity by Ostwald Viscometer

- To discuss the effect of temperature on surface tension and coefficient of viscosity.

Solids

- To discuss different forms of solids, symmetry elements, unit cells and crystal systems.
- To discuss Bravais lattice systems.
- To explain the laws of crystallography.

Learning Outcomes:

The students will be able to:

1. Understand the periodicity in atomic and ionic radii, electronegativity, ionization energy, electron affinity of elements of the periodic table.
2. Understand the chemistry of s and p-block elements.
3. Understand Oxidation states with reference to elements in unusual and rare oxidation states like carbides and nitrides.
4. Predict the formula and the name of simple compounds of s- and p-block elements.
5. Explain the stability of common oxidation state for s and p block element of s & p-block of each groups.
6. Understand the anomalous behaviour of the first elements.
7. Understand vital role of Sodium, Potassium, Calcium and magnesium in biological system
8. Understand the use of Cesium in devising photoelectric cells, use of radium salts in radiotherapy

The student will be able to

1. Understand the kinetic theory of gases and derive gas laws from it.
2. Gain on understanding the 'gas laws' governing the physical behaviour of gases
3. Know the reason for deviation of real gases from ideal behavior
4. Predict the necessary conditions for liquefaction of gases
5. Explain the various factors affecting viscosity of gases
6. Understand the surface tension and viscosity of liquids and various factors affection them
7. Appreciate the daily life experiences related with surface tension and viscosity
8. Carryout experiments to determine surface tension and viscosity
9. Classify different types of solids and their basic structure.
10. Appreciate the laws of crystallographyfor determining the geometry and fine structure of crystals

Unit 1:

Section A -- Inorganic Chemistry **(Lectures-30)**

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, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, van Arkel-de Boer process. Mond's process and Zone Refining.

(4 Lectures)

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, Winker), 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

(26 Lectures)

Unit 3:

Physical Chemistry **(30 Lectures)**

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 CO2.
- 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).

(10 Lectures)

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) .

(3 Lectures)

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.

(6 Lectures)

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, liragg's law. Structures of NaI, KCI and CsCI (qualitative treatment only). Defects in crystals. Glasses and liquid crystals.

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).

(11 Lectures)

Practical:

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+} , 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-} , $C_2O_4^{2-}$.
(Spot tests should be carried out wherever feasible)

Section B: Physical Chemistry

(I) Surface tension measurement (use of organic solvents excluded).
a) Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.
b) Study of the variation of surface tension of a detergent solution with concentration.
(II) 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.
(III) Chemical Kinetics
Study the kinetics of the following reactions by integrated rate method:
a) Acid hydrolysis of methyl acetate with hydrochloric acid.
b) Saponification of ethyl acetate.
Rqference.Boolcs:
•A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
. B.D. Khosla, Practical Chemistry

References:

Theory:

- Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 3 rd Ed.(adapted), Pearson, 2009 ISBN 978-81-31718858

Practical:

- G. M. Barrow: Physical Chemistry Tata McGraw Hill (2007).
- G. W. Castellan: Physical Chemistry 4th Edn. Narosa (2004).
- J. C. Kotz, P. M. Treichel& J. R. Townsend: General Chemistry Cengage Lening India Pvt. Ltd., New Delhi (2009).
- B. H. Mahan: University Chemistry 3rd Ed. Narosa (1998).
- R. H. Petrucci: General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985),
- J. D. Lee: A New Concise Inorganic Chemistry, E.L.B.S.
- F.A. Cotton & G. Wilkinson: Basic Inorganic Chemistry, John Wiley.
- D. F. Shriver and P. W. Atkins: Inorganic Chemisity, Oxford University Press.
- Gary Wulfsberg: Inorganic Chemistry, Viva Books Pvt. Ltd.
- Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 3rd Ed (adapted), Pearson, 2009 ISBN 978-81-31718858.

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
- To provide latest knowledge and skills to students.
- Correlating the topic with real life cases.
- Quiz contest should be carried out among some important topic of syllabus

Assessment Methods:

To encourage students to visit one factory and prepare a report on that visit.

- Through assignment and test.
- To encourage students to prepare salient feature of the topic given by teacher and assessing them.
- Quizzes·
- Response of individual student throughout the year and at the end of class .
- Presentations.

- Essays.
- To write an article that is graded for content and style.

Keywords

Metallurgy,Periodicity,Anomalous behaviour , Ellingham diagrams, Hydrometallurgy , Periodicity , Allotrophy, Diagonal relationship, Multicentre bonding , Kinetic Theory, Arrhenius Equation, Bravais Lattice, Miller indices, Bragg's law, Surface tension, Viscosity, Maxwell Boltzmann Distribution law, Andrews equation.Qualitative Analysis, Chemical Kinetics.

Chemistry of d-Block Elements, Quantum Chemistry and Spectroscopy (Chemistry GE v)

CHEMISTRY GE- v
Total Credits: 06 **(Credits: Theory-04, Practicals-02)**
(Total Lecture: Theory- 60, Practicals-60)

Objectives:

The students will be able to:

Inorganic (Section A):

The course introduces 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 also familiarizes them with coordination compounds which find manifold applications in diverse fields.

Physical (Section B):

The objective of this course is to familiarize the student

1. With the concepts and methodology of quantum mechanics.
2. Its applications to spectroscopy.
3. Basic knowledge of relation between structure determination and spectra.

Learning Outcomes:

The student is expected to learn/understand the following:

1. Properties of d and f block elements
2. Latimer Diagrams
3. Properties of coordination compounds
4. VBT and CFT for bonding in coordination compounds
5. Basic principles of quantum mechanics : operators, eigen values, averages, probability distributions.
6. Quantisation of translational, rotational and vibrational energies
7. Basic concepts of microwave, IR and UV-VIS spectroscopy
8. Lambert Beer's Law, quantum efficiency and photochemical processes.

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.

(10 Lectures)

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.

(6 Lectures)

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.

(14 Lectures)

Unit 4:

Quantum Chemistry

1. Postulates of quantum mechanics, quantum mechanical operators.
2. Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wave functions, concept of zero-point energy.
3. Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.
4. Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels

(12 Lectures)

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**.**

(12 Lectures)

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.

(6 Lectures)

Practical:

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 λmax 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

- Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration
- Analyse the given vibration-rotation spectrum of HCl(g)

References:

- G. M. Barrow: Physical Chemistry Tata McGraw---Hill (2007).
- J. C. Kotz, P. M. Treichel& J. R. Townsend: General Chemistry, Cengage Lening India Pvt. Ltd., New Delhi (2009).
- B. H. Mahan: University Chemistry 3rd Ed. Narosa (1998).
- J. D. Lee: A New Concise Inorganic Chemistry, E.L.B.S.
- F.A. Cotton & G. Wilkinson: Basic Inorganic Chemistry, John Wiley.
- Gary Wulfsberg: Inorganic Chemistry, Viva Books Pvt. Ltd.
- A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- A.I. Vogel, Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

Additional Resources:

- G. W. Castellan: Physical Chemistry 4th Edn. Narosa (2004).
- R. H. Petrucci: General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985).
- D. F. Shriver and P. W. Atkins: Inorganic Chemistry, Oxford University Press.

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:

There should be a multi-pronged approach for evaluating a student's understanding of the key concepts. Some of the methods that can be used are:

- Class assignments
- Short quiz
- Presentations

Keywords:

d block, actinoids, lanthinoids, VBT, crystal field theory, splitting of d levels, coordination compounds, quantisation, selection rules, Schrodinger equation, operator, spectrum, quantum efficiency, fluorescence.

Organometallics, Bioinorganic Chemistry, Biomoleculesand UV, IR Spectroscopy
(Chemistry GE vi)

CHEMISTRY GE- vi

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

Objectives:

The purpose of the course is to introduce students of Honours courses other than Chemistry 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 topics of carbohydrates ,Aminoacids ,Peptides and proteinsare introduced through some specific examples. A relationship between structure,reactivity and biological properties of biomolecules is established through the study of these representative biomolecules. The learners are introduced to Spectroscopy, an important analytical tool which allows identification of organic compounds without the aid of reagents.

Learning Outcomes:

On completion of the course, the student will be able to:

- Understand the chemistry of the different oxidation states of 3d metals
- Get an idea of the preparation and important properties of the familiar compounds potassium dichromate, potassium permanganate and potassium ferrocyanide
- Bonding in organometallic compounds
- Use IR data to explain the extent of back bonding in carbonyl complexes
- Recognize the role of metal ions present in biological systems with special reference to Na^+, K^+, Mg^{2+}, Fe ions
- Get a general idea of toxicity of metal ions through the study of Hg^{2+} and Cd^{2+} in the physiological system
- Understand and demonstrate how the structure of biomolecules determines their chemical properties,reactivity and biological uses.
- Gain insight intothe basic fundamental principles of IR and UV-Vis spectroscopic techniques.

- Use basic theoretical principles underlying UV-visible and IR spectroscopy for qualitative organic analysis of functional groups.

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

(6 lectures)

Unit 2:

Organometallic Compounds

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

(12 Lectures)

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+}).

(12 lectures)

Unit 4:

Amino Acids, Peptides and Proteins:

Zwitterion, Isoelectric point and Electrophoresis

Preparation of Amino Acids: Strecker synthesis using Gabriel's phthalimide synthesis.

Reactions of Amino acids: ester of –COOH group, acetylation of –NH2 group, complexation with Cu2+ 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.

(10 Lectures)

Unit 5:

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 disacharrides (sucrose, cellobiose, maltose, lactose) and polysacharrides (starch and cellulose) excluding their structure elucidation.

(8 Lectures)

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).

(12 Lectures)

Practical:

Section A: Inorganic Chemistry

1. Separation of mixtures of two ions by paper chromatography and measurement of *Rf* value in each case:
Fe^{3+}, $A1^{3+}$ and Cr^{3+} or Ni^{2+}, Co^{2+}, Mn^{2+} and Zn^{2+}
2. Preparation of the following complexes and measurement of their conductivity:
(i) Tetraamminecopper(II) sulphate
(ii) Potassium trioxalatoferrate(III) trihydrate

Section B: Organic Chemistry

1. Identification of simple organic compounds containing the above functional groups by IR spectroscopy through examination of spectra (spectra to be provided).
2. Estimation of Glycine by Sorenson's Formol titration
3. Systematic qualitative analysis of organic compounds possessing monofunctional groups:, nitro, amide,amines, carbohydrates (excluding derivative preparation)

References:

Theory:

- James E. Huheey, Ellen Keiter& Richard Keiter: *Inorganic Chemistry: Principles of* Structure and Reactivity, Pearson Publication
- G.L. Miessler& Donald A. Tarr: *Inorganic Chemistry,* Pearson Publication
- J.D. Lee: A New Concise Inorganic Chemistry, E.L.B.S
- I.L. Finar: *Organic Chemistry* (Vol. I & II), E.L.B.S
- Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry,* S. Chand.
- John R. Dyer: Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall.

Practical:

- V.K. Ahluwalia, Sunita Dhingra and Adarsh Gulati: College Practical Chemistry,
- University Press (India) Ltd. (2005).
- V.K. Ahluwalia & Sunita Dhingra: Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).
- A.I. Vogel: Textbook of Practical Organic Chemistry, Prentice Hall, 5th Ed.
- F. G. Mann & B. C. Saunders: Practical Organic Chemistry, Orient Longman (1960).

Additional Resources:

- F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley & Sons.
- R.M. Silverstein, G.C. Bassler& T.C. Morrill*: Spectroscopic Identification of Organic Compounds*, John Wiley & Sons.

- R.T. Morrison & R.N. Boyd: *Organic Chemistry,* Prentice Hall.
- Peter Sykes: A Guide Book to Mechanism in Organic Chemistry, Orient Longman.

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

Molecules of Life

Chemistry GE (vii) **Total Credits: 06**

(Credits: Theory-04, Practicals-02)

(Total Lecture: Theory- 60, Practicals-60)

Objectives:

1. 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 biomolecules.
2. To extend the knowledge of synthetic organic chemistry to chemistry of biomolecules
3. Key emphasis is placed on understanding the structural principles that govern reactivity/physical /biological properties of biomolecules as opposed to learning structural detail.

Course Learning Outcomes:

1. Students will be able to understand and demonstrate how the structure of biomolecules determines their chemical properties ,reactivity and biological uses.
2. The students will gain an insight into mechanism of enzyme action and inhibition.
3. The students will understand the basic principles of drug-receptor interaction and SAR.
4. The students gain an insight into biological processes like replication ,transcription and translation .
5. Students will be able to 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. 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.

(10 Lectures)

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 (upto 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.

(12 Lectures)

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 stereospecifity) , Enzyme inhibitors and their importance, phenomenon of inhibition(Competitive and Non competitive inhibition including allosteric inhibtion). Drug action-receptor theory. Structure – activity relationships of drug molecules, binding role of –OH group,-NH2 group, double bond and aromatic ring.

(10Lectures)

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.

(10 Lectures)

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).

(8 Lectures)

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.

(8 Lectures)

Practical:

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:

- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Berg, J. M., Tymoczko, J. L. &Stryer, L. Biochemistry 7th Ed., W. H. Freeman.

Practical:

- Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, ELBS.
- Introduction to Practical Biochemistry by S K Swahney and RandhirSingh,Nerosa Publications.
- Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.
- Arthur, I. V. Quantitative Organic Analysis, Pearson.

Teaching Learning Process:

- The teaching learning process will involve the traditional chalk and black board method.
- 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 curriculumbased topics.
- As the best way to learn something is to do it yourself, practicals are planned in such a way so as to reinforce the topics covered in theory.

Assessment Methods:

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

Keywords:

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

New Course Additions

CHEMISTRY-CC/DSE: **Nano Dimensional Materials and Their Applications**

Marks: 100 Duration: 60 Hours (4 credits)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Course Objective: Thecourse opens the arena of nanodimensions to the students. It will help the students to appreciate the real life applications of nanomaterials. It will alsodevelop their interest in the research area of materials chemistry.

Course Learning Outcomes:

Upon successful completion of the course, the students would be able to:

1. Understand the concept of nanodimensions.
2. Know the various synthetic methods used for the preparation of nanomaterials.
3. Know the different characterization techniques used for the analysis of nanomaterials and understand the basic principle behind these techniques.
4. Discuss the optical and conducting properties of nanostructures.
5. Appreciate the real life applications of nanomaterials.

Content:

Unit-1

INTRODUCTION TO NANODIMENSIONS: 0D, 1D, 2D nanomaterials, Quantum Dots,Nanoparticles, Nanostructures (nanowires, thin films, nanorods), carbon nanostructures (carbon nanotubes, carbon nanofibers, fullerenes), Size Effects in nano systems, Quantum confinement and its consequences, Semiconductors.Band structure and band gap.(10 Lectures)

Unit-2

SYNTHESIS OF NANO MATERIALS: Top down and Bottom up approach, Photolithography. Ball milling.Vacuum deposition.Physical vapor deposition (PVD), Chemical vapor deposition (CVD), Thermal evaporation, Pulsed Laser deposition.Sol-Gel Synthesis, Electrochemical deposition, Spray pyrolysis,Hydrothermal synthesis. Preparation through colloidal methods. Self-assembled growth of nanostructures,Molecular beam epitaxy (MBE) growth of quantum dots. (8 Lectures)

Unit-3

CHARACTERIZATION: X-Ray Diffraction (Powder and Single Crystal). Scanning Electron Microscopy (SEM).Transmission Electron Microscopy (TEM).Atomic Force Microscopy (AFM).Scanning Tunneling Microscopy (STM). Dynamic light scattering (DLS), Brunauer-Emmett-Teller (BET) Surface area measurement. (8 Lectures)

Unit- 4

OPTICAL PROPERTIES: Excitons in direct and indirect band gap semiconductor nanocrystals. Radiative processes: General absorption, emission and luminescence (fluorescence and photoluminescence). (14 Lectures)

Unit-5

CONDUCTING PROPERTIES: Carrier transport in nanostructures.Tunneling and hoping conductivity. Defects and impurities: Deep level and surface defects. (6 Lectures)

Unit-6

APPLICATIONS: Applications of nanoparticles, quantum dots, nanowires and thin films for photonic devices (LEDs, solar cells, transistors). Nanomaterial Devices. CNT based transistors. Quantum dots heterostructure lasers. (14Lectures)

Reference books:

- A.R. West, Solid State Chemistry, (Wiley India Pvt. Ltd.).

- C.N.R. Rao, New Directions in Solid State Chemistry
- Smart and Moore, Solid State Chemistry
- C.P.Poole, Jr. Frank J.Owens, Introduction to Nanotechnology (Wiley India Pvt. Ltd.).
- S.K. Kulkarni, Nanotechnology: Principles & Practices (Capital Publishing Company)
- K.K. Chattopadhyay and A. N. Banerjee, Introduction to Nanoscience and Technology (PHI Learning Private Limited).
- Introduction to Nanoelectronics, V.V. Mitin, V.A. Kochelap and M.A. Stroscio, 2011, Cambridge University Press.
- Richard Booker, Earl Boysen, Nanotechnology (John Wiley and Sons).

PRACTICALS:

Nano Dimensional Materials and their Applications

Marks: 50 Durations: 60 Hours (2 credits)

At least 04 experiments from the following:

1. Synthesis of metal nanoparticles by chemical route.

2. Synthesis of semiconductor nanoparticles.

3. Surface Plasmon study of metal nanoparticles by UV-Visible spectrophotometer.

4. XRD pattern of nanomaterials and estimation of particle size.

5. To study the effect of size on color of nanomaterials.

6. To prepare composite of CNTs with other materials.

7. Growth of quantum dots by thermal evaporation.

8. Prepare a disc of ceramic of a compound using ball milling, pressing and sintering, and study its XRD.

9. Fabricate a thin film of nanoparticles by spin coating (or chemical route) and study transmittance spectra in UV-Visible region.

Reference Books:

- C.P.Poole, Jr. Frank J.Owens, Introduction to Nanotechnology (Wiley India Pvt. Ltd.).
- S.K. Kulkarni, Nanotechnology: Principles & Practices (Capital Publishing Company).
- K.K. Chattopadhyay and A.N. Banerjee, Introduction to Nanoscience & Technology (PHI Learning Private Limited).
- Richard Booker, Earl Boysen, Nanotechnology (John Wiley and Sons)

CHEMISTRY GE/SEC- **Renewable Energy and Solar Photovoltaics: Principles, Technologies & Materials**

Marks: 100 Duration: 60 Hours (4 credits)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Course Objective:

To introduce renewable energy sources, the various technologies of harnessing them and how to save the energy captured through energy efficiency.

Course Learning Outcomes:

Upon successful completion of the course, the students will be able to:

- To give a structured overview of the different renewable energy sources, how they can be harnessed and used for the provision of electricity, heat and cold.
- To present the different systems, their components, how they are designed and work
- Describe how each technology works
- Undertake initial system designs and sizing
- Analyze the renewable energy markets and latest market trend

Content:

Unit-1

Global Energy Scenario:

Discovery of various energy sources: Energy Sources and Overall Energy demand and availability, Energy Consumption in various sectors and its changing pattern, Exponential increase in energy consumption and Projected future demands.

Energy Resources: Coal, Oil, Natural Gas, Nuclear Power and Hydroelectricity, Solar and Other Renewable etc. Depletion of energy sources and its impact.

Future Energy Options: Sustainable Development, Energy Crisis: Transition from carbon rich and nuclear to carbon free technologies, parameters of transition.

Energy Policy Issues: Fossil Fuels, Renewable Energy, Power sector reforms, restructuring of energy supply sector, energy strategy for future. (10 Lectures)

Unit-2

Energy Conversion Systems-

Principle fuels for energy conversion: Fossil fuels, Nuclear fuels. Conventional & Renewable Energy

Energy Sources: prospecting, extraction and resource assessment and their peculiar characteristics.

Conversion of chemical energy into electrical energy (fuel cell).

Thermal power plant, nuclear power plants and hydroelectric power plant, Transmission and distribution of electricity, Villages electrification program and problems in India. (10 Lectures)

Unit-3

Solar Energy : Sun as Source of Energy, Availability of Solar Energy, Nature of Solar Energy, Solar Energy & Environment. Various Methods of harvesting solar energy –Photothermal, Photovoltaic, Photosynthesis, Present & Future Scope of Solar energy.

Solar Radiation : Nature of Solar Radiation, Estimation of Solar Radiation, Measurement of Solar Radiation. (10 Lectures)

Unit-4

Solar Technologies:

Semiconductors, Introduction to Band Theory, Electrical Properties of Semiconductors.Essential characteristics of solar photovoltaic devices. First Generation Solar Cells, Second Generation Solar Cells, Solar Cell Device Parameters.

Photo thermal Systems:Various Collectors and Solar Concentrators, Central Receiver System, Solar Water Heating Systems(Active & Passive), Solar Space Heating & Cooling Systems, Solar Dryers & Desalination Systems.

Photovoltaic systems : Solar cells & panels, performance of solar cell, estimation of power obtain from solar power, solar panels PV systems, applications of PV systems, concentrating PV systems, PV power plants.

Third Generation Solar Cells: Organic and Dye Sensitized Solar Cells, Perovskite Solar Cells.

(22 Lectures)

Unit-5

Economic analysis of Solar energy Systems : Life cycle analysis of Solar Energy Systems, Time Value of Money, Evaluation of Carbon Credit of Solar Energy Systems. (8 Lectures)

Reference Books:

1. Energy for a sustainable world: Jose Goldenberg, Thomas Johansson, A.K.N.Reddy, Robert Williams (Wiley Eastern).

2. TEDDY Year Book Published by Tata Energy Research Institute (TERI),

3. World Energy Resources : Charles E. Brown, Springer2002.

4. Handbook of Photovoltaic Science and Engineering. Eds. A. Luque and S. Hegedus, Wiley

5. Direct Energy Conversion :W.R.Corliss

6. Aspects of Energy Conversion :I.M.Blair and B.O.Jones

7. Principles of Energy Conversion :A.W.Culp (McGrawHill International)

8.Solar Engineering of Thermal Process, J.A.Duffie& W.A. Beckman, Wiley.

9. Solar Energy Engineering, S.A.Kalogirou, Elsevier 2009

Practical-

Renewable Energy and Solar Photovoltaics: Principles, Technologies & Materials

Mars: 50 Durations: 60 Hours (2 credits)

Atleast04practicals should be done during a semester.

1. Measurement of Intensity of solar radiation.

2. Energy Content in Wind. (Prototype Wind Mill of 500W)

3. Bio-gas Production from Kitchen waste.

4. Study of solar collector.

5. Study of solar hot water systems (FPC and ETC)

6. Study of solar hot air collector/ solar dryer.

7. Performance evaluation of box type and concentrating type solar cooker.

8. Study of Chulla and Gas Stove.

9. Study of Lead Acid Battery as an energy storage.

10. Study of Performance of Solar Lamp.

11. Wind power and annual energy estimation from wind data.

12. Solar power and annual energy estimation from given data.

13. Pay back analysis, financial work sheet of a renewable energy project.

Reference Books:

1. Energy for a sustainable world: Jose Goldenberg, Thomas Johansson, A.K.N.Reddy, Robert Williams (Wiley Eastern).

2. Handbook of Solar Energy: Theory, Analysis and Applications (Energy Systems in Electrical Engineering) 1st ed. 2016 Edition, Kindle Edition

by G. N. Tiwari, Arvind Tiwari, Shyam

3. Principles of Energy Conversion: A.W.Culp(McGrawHill International)

4. Solar Engineering of Thermal Process, J.A.Duffie& W.A. Beckman, Wiley.

5. Solar Energy Engineering, S.A.Kalogirou, Elsevier 2009

6. Organic Photovoltaics,Editor(s): Dr. Christoph Brabec Prof. Dr. Vladimir Dyakonov Prof. Dr. Ullrich Scherf, by Wiley

7. Solar Energy: Fundamentals, Technology, and Systems, Klaus Jäger, Olindo Isabella, Arno H.M. Smets, René A.C.M.M. van Swaaij, Miro Zeman, Delft University of Technology, 2014

Evaluation:

Class Test, Assignment, Project Work, Field Visit, Presentation etc.

Generic Elective Course

GREEN CHEMISTRY: DESIGNING CHEMISTRY FOR HUMAN HEALTH AND ENVIRONMENT

CHEMISTRY GE (i)
Total Credits: 06 (Credits: Theory-04, Practicals-02)
(Total Lecture: Theory- 60, Practicals-60)

Objectives:

Brief Background and significance of introducing this course *(This description is provided because this course is being floated for the first time).*

Undeniably, chemical products and processes are central to global economy as they have been playing an indispensable role in not only meeting our fundamental needs for food, shelter and clothing and but also benefitting us in numerous other ways through various technological advancements. However, these benefits have come at an enormous price. Most of the chemical processes have led to the generation of toxic waste materials that have migrated to various environmental matrices and caused a detrimental impact on human health. Therefore, this grave situation has made us re-think of ways in which we have been practising chemistry and raised crucial questions:

1. ***How can we strengthen the economy, protect the environment and ensure a high quality of life?***

2. ***How can we educate succeeding generations of chemists so that they will have the skills and knowledge to practice chemistry in ways that are benign to human health and environment?***

It is here where green chemistry comes into picture. But the successful outcomes of practising green chemistry cannot be realized only with chemists; intervention of engineers, economists, ecologists, toxicologists, policy makers is also essential. For instance: a chemical engineer can design a production line to recycle certain reagents and minimize energy consumption. Toxicologists and ecologists provide information about the toxic characteristics and effect of molecules so that the chemists can work to design new molecules that avoid structures linked to toxicity.

This course reflects the power that a green chemist not only holds over the disposition of the chemistry that is created, from its creation, to its use, until its destruction and beyond. Beyond, because a chemist can not only design a substance to have certain characteristics during its useful life, but can also design what substance will become (or break down) after its useful life is over.

Students at all levels can benefit from an introduction to Green Chemistry. This course aims at:

1. Raising an awareness on the potential toxic effects of different chemicals and problems related to waste generation.
2. Inculcating the need to practice green chemistry as it is the only way to meet the global challenges the world is facing today. Green Chemistry possesses the potential to reduce waste generation and enhances our quality of lives while conferring simultaneous benefits of protecting our environment and human health.
3. Providing a basis and framework for pursuing science in the most creative, innovative and responsible manner possible.
4. Familiarizing students with the new emerging green technologies (new catalysts, solvents and energy sources) that would help them gain new insights on how pollution can be prevented through thoughtful design of chemical products and processes.
5. Enabling students to learn about the green trends being practiced by industries as well as academicians through demonstration of some real world case studies.
6. Enabling the next generation to learn from the concepts reflected in this course that perhaps one day green chemistry will not be an additional consideration when designing a synthetic route or industrial process.

Learning Outcomes:

After studying this course, students will be able to:

- Understand what is waste and how waste generation can give cause serious repercussions on our environment while simultaneously causing enormous damage to human health.
- Recognize and acknowledge the role of green chemistry in reducing waste, learn about new strategies (emerging green technologies-green catalysts, solvents, energy, plastics etc.) that possess tremendous potential in reducing waste
- Creatively redesign traditional experiments with a green focus (using the various principles of green chemistry)
- Learn about the green trends being practiced in pharmaceutical industries through depiction of some interesting industrial case studies
- Learn about academic-industrial collaborations and the potential these relationships hold in furtherance of green chemistry and rendering our planet earth greener
- Eliminate “Do as I Said attitude” of students as this course will enhance the creative practical skills of students
- Motivate students to choose discipline and career related to this field. Eventually a student practising green chemistry can either become an industrialist or engineer or policy maker.

Unit 1:

Waste: Production & Problems

Green Chemistry: The perfect toolbox to prevent waste

- Twelve Principles of Green Chemistry
- Special Emphasis on Prevention of Waste

(8 Lectures)

Unit 2:

Accelerating Innovations through Emerging Green Technologies

3.1 Green Energy

3.1.1 Global Warming (Climate Change)

3.1.2 Renewable energy

Solar Power- Other forms of renewable energy

3.1.3 Microwave Assisted Synthesis

3.1.4 Ultrasound Assisted Synthesis

3.2 Green Solvents

3.2.1 Problems associated with traditional solvents

3.2.2 Water as a green solvent

3.2.3 Ionic Liquids

3.2.4 Bio-based Solvents

3.2.5 Supercritical CO_2

3.3 Green Catalysts

3.3.1 General Introduction to Catalysis

3.3.2 Types of Catalysts

3.3.3 Green Catalyst

3.3.4 Nanocatalyst **(17 Lectures)**

Unit 3:

Green Chemistry solutions for water pollution *(Current Green Technologies employed in Water Treatment)*

4.1 Water Pollution and root causes

4.2 Catalytic Degradation of organic water pollutants

4.3 Photo-oxidation technologies

4.4 Removal of heavy metals (inorganic pollutants) via new adsorption technology

(10 Lectures)

Unit 4:

Green Chemistry in Pharmaceutical Industry

- Green Trends being followed in pharma
- Industrial Case Studies
  - *Ranitidine*
  - *Celecoxib*
  - *Ibuprofen*
  - *Sertraline*
- Special Recognition: US Presidential Green Challenge Awards

(10 Lectures)

Unit 5:

New Directions from Academia

- Innovations stemming from academia
- Academia Being Recognized: US Presidential Green Challenge Awards

(5 Lectures)

Unit 6:

Green chemistry and resource efficiency: towards a green circular economy

- Resource efficiency, atom economy and the *E* factor
- Concept of Circular Economy: Renewable resources, the bio-based economy and waste valorisation
- Creating an Effective Regulatory System
- New Technological Developments: New Avenues for the Green Economy and Sustainable Future of Science and Technology

Future Prospectives **(10 Lectures)**

Practical:

Green Chemistry experiments need to be designed with the help of the three magic R's- Reduce, Reuse and Recycle.

While designing and practising green chemistry experiments, special emphasis should be made on utilizing the maximum tenets (principles) of Green Chemistry:

- **GETTING OFF TO A SAFE START:** Using Safer Starting Materials for Chemical Reactions
- **AIM AT DESIGNING GREEN SYNTHETIC PATHWAYS:** Involves safe solvents (for instance: liquid co_2, ionic liquids, water) and green reaction conditions.
- **AVOIDING WASTE:** Maximizing Atom Economy
- **CONSERVING ENERGY:** Using Lower Amounts of energy for chemical processes
- **GREENING WASTES:** Returning safe substances to the environment

Practical applications (Experiments to be performed):

(I) Converting Waste to Wealth:

- Synthesis of biodiesel from waste cooking oil

(II) Using Renewable resources for deriving valuable products:

- Making green plastics from corn starch

(III) Greener approach to the synthesis of Gold/Silver Nanoparticles:

- Green synthesis of gold/silver nanoparticles

(IV) Degradation of toxic pollutants (dyes):

- Catalytic degradation of dyes using nanoparticles (can be any)

(V) Green Synthesis

- Microwave assisted synthesis of copper phthalocyanine complex
- Preparation of Fe(III)AcAc Complex using a greener approach

References:

Theory:

- P.T. Anastas & J. C. Warner, Green Chemistry: Theory and Practice (1998), Oxford University Press.
- M. Lancaster, Green Chemistry: An Introductory Text RSC Publishing (2010), 2nd Edition, ISBN-978-1-84755-873-2.
- M. C. Cann & Thomas P. Umile, Real-World Cases in Green Chemistry Vol II (2008), American Chemical Society.
- M. C. Cann & M. E. Connelly, Real-World Cases in Green Chemistry

- R. K. Sharma & R. Bandichhor, Hazardous Reagent Substitution (2018), Royal Society of Chemistry.
- K. Parent & M. Kirchhoff, Going Green: Integrating Green Chemistry into the Curriculum (2004), American Chemical Society.

Practical:

- R. K. Sharma, I. T. Sidhwani & M. K. Chaudhuri, Green Chemistry Experiments: A Monograph (2007), Tucker Prakashan.
- Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, Department of Science and Technology, Government of India. http://dst.gov.in/green-chem.pdf.
- M. Kirchhoff & M. A. Ryan, Greener Approaches to Undergraduate Chemistry Experiments (2002), American Chemical Society.
- M. S. Ryan & M. Tinnesand, Introduction to Green Chemistry (2002), American Chemical Society.

Teaching Learning Process:

- Interactive Classes
- Experiential Learning
- Power point presentations
- Visit to pharmaceutical industries and green chemistry laboratories
- Interesting and inspiring short videos and movies in green chemistry
- Activities related to green chemistry would be conducted in classrooms that would enhance the critical thinking of students and help them redesign experiments in a greener way

Assessment Methods:

Following **assessment methods** can be adopted to evaluate the students:

- Conventional Class tests
- Open Book tests
- Assignments
- Online tests --objective or subjective
- Quizzes
- Presentation on a topic in front of the classmates
- Performing a new experiment based on the concepts learned in the course.

Keywords:

Waste production, problem and prevention; Emerging green technologies, Green Catalysts, Green Solvents, Green Energy, photo-oxidation technologies, industry-academia collaboration, circular economy

.