

B.SC. LIFE SCIENCE

CHEMISTRY COURSES OFFERED UNDER B.Sc. Life Science PROGRAMME (CBCS)

CORE COURSES (six credits each) – Each course has 4 Periods/week for Theory, 4 Periods/week for Practical			
SEMESTER	COURSE CATEGORY	NAME OF THE COURSE	CREDITS T=Theory Credits P=Practical Credits
I	CORE	Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons	T=4 P=2
II	CORE	Chemical Energetics, Equilibria and Functional Group Organic Chemistry-I	T=4 P=2
III	CORE	Solutions, Phase Equilibrium, Conductance, Electrochemistry and Functional Group Organic Chemistry-II	T=4 P=2
IV	CORE	Chemistry of s- and p-Block Elements, States of Matter and Chemical Kinetics	T=4 P=2

DISCIPLINE SPECIFIC ELECTIVE (DSE) (SIX credits each)**Two courses (Chemistry of d-block elements, Quantum Chemistry and Spectroscopy and any one from the rest) are offered in Semester V/VI**

COURSE CATEGORY	NAME OF THE COURSE	CREDITS T=Theory Credits P=Practical Credits
CHEMISTRY DSE-1	Applications of Computers in Chemistry	T=4 P=2
CHEMISTRY DSE-2	Analytical Methods in Chemistry	T=4 P=2
CHEMISTRY DSE-3	Molecular Modelling & Drug Design	T=4 P=2
CHEMISTRY DSE-4	Novel Inorganic Solids	T=4 P=2
CHEMISTRY DSE-5	Polymer Chemistry	T=4 P=2
CHEMISTRY DSE-6	Research Methodology for Chemistry	T=4 P=2
CHEMISTRY DSE-7	Green Chemistry	T=4 P=2
CHEMISTRY DSE-8	Industrial Chemicals & Environment	T=4 P=2
CHEMISTRY DSE-9	Inorganic Materials of Industrial Importance	T=4 P=2
CHEMISTRY DSE-10	Instrumental Methods of Chemical Analysis	T=4 P=2
CHEMISTRY DSE-11	Chemistry of d-block elements, Quantum Chemistry and Spectroscopy (compulsory)	T=4 P=2
CHEMISTRY DSE-12	Organometallics, Bioinorganic chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy	T=4 P=2
CHEMISTRY DSE-13	Molecules of Life	T=4 P=2
CHEMISTRY DSE-14	Nanoscale Materials and their Applications	T=4 P=2
CHEMISTRY DSE-15	Dissertation	6

Skill Enhancement Courses (SEC) (four credits each) Any four courses from the following to be offered in Semester III/IV/V/VI		
COURSE CATEGORY	NAME OF THE COURSE	CREDITS T=Theory Credits P=Practical Credits
CHEMISTRY SEC-1	IT Skills for Chemists	T=4 P=2
CHEMISTRY SEC-2	Basic Analytical Chemistry	T=4 P=2
CHEMISTRY SEC-3	Chemical Technology & Society	T=4 P=2
CHEMISTRY SEC-4	Cheminformatics	T=4 P=2
CHEMISTRY SEC-5	Business Skills for Chemists	T=4 P=2
CHEMISTRY SEC-6	Intellectual Property Rights	T=4 P=2
CHEMISTRY SEC-7	Analytical Clinical Biochemistry	T=4 P=2
CHEMISTRY SEC-8	Green Methods in Chemistry	T=4 P=2
CHEMISTRY SEC-9	Pharmaceutical Chemistry	T=4 P=2
CHEMISTRY SEC-10	Chemistry of Cosmetics & Perfumes	T=4 P=2
CHEMISTRY SEC-11	Pesticide Chemistry	T=4 P=2
CHEMISTRY SEC-12	Fuel Chemistry	T=4 P=2

Student has to study 4 core papers in chemistry in semesters I, II, III & IV.

Student has to study 4 Skill Enhancement Courses (SEC), which can be chosen from Chemistry/Botany/Zoology. (At least ONE SEC of each discipline)

Student has to study 2 Discipline Specific Elective papers from Chemistry in semester V & VI.

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

SEMESTER –I

Course Code: CHEMISTRY – Core Paper-1

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

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

Section A: Inorganic Chemistry (Lectures:30)

Unit 1:

Atomic Structure

Review of: Bohr's theory and its limitations, Heisenberg uncertainty principle, Dual behaviour of matter and radiation, De-Broglie's relation, Hydrogen atom spectra, need of a new approach to atomic structure. What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of ψ and ψ^2 , Schrödinger equation for hydrogen atom, radial and angular parts of the hydrogenic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation), radial and angular nodes and their significance, radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals.

Significance of quantum numbers, orbital angular momentum and quantum numbers m_l and m_s . Shapes of s, p and d atomic orbitals, nodal planes, discovery of spin, spin quantum number (s) and magnetic spin quantum number (m_s).

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

(Lectures: 14)

Unit 2:

Chemical Bonding and Molecular Structure

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

Covalent bonding: VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR (H_2O , NH_3 , PCl_5 , SF_6 , ClF_3 , SF_4) and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.

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

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

(Lectures: 16)

Section B: Organic Chemistry (Lectures:30)

Unit 3:

Fundamentals of Organic Chemistry

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

(Lectures: 08)

Unit 4:

Stereochemistry

Conformations with respect to ethane, butane and cyclohexane, interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations, concept of chirality (upto two carbon atoms). configuration: geometrical and optical isomerism; enantiomerism, diastereomerism and meso compounds). Threo and erythro; D and L; *cis-trans* nomenclature; CIP Rules: R/ S (for upto 2 chiral carbon atoms) and E / Z nomenclature (for upto two C=C systems).

(Lectures: 10)

Unit 5:

Aliphatic Hydrocarbons

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

Alkanes:

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

Reactions: Free radical substitution: Halogenation.

Alkenes:

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

Reactions: cis-addition (alk. KMnO_4) and trans-addition (bromine), addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymercuration-demercuration, Hydroboration-oxidation.

Alkynes:

Preparation: Acetylene from CaC_2 and conversion into higher alkynes; by dehalogenation of tetrahalides and dehydrohalogenation of vicinal-dihalides.

Reactions: formation of metal acetylides and acidity of alkynes, addition of bromine and alkaline KMnO_4 , ozonolysis and oxidation with hot alk. KMnO_4 . Hydration to form carbonyl compounds

(Lectures: 12)

Practical:

(Credits: 2, Laboratory periods: 60)

Section A: Inorganic Chemistry - Volumetric Analysis

1. Estimation of oxalic acid by titrating it with KMnO_4 .
2. Estimation of Mohr's salt by titrating it with KMnO_4 .
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO_4 .
4. Estimation of Fe (II) ions by titrating it with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $\text{Na}_2\text{S}_2\text{O}_3$.

Section B: Organic Chemistry

1. Purification of organic compound by crystallisation (from water and alcohol) and distillation.
2. Criteria of purity: Determination of M.P./B.P.

3. Separation of mixtures by chromatography: Measure the 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:

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

Practical:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords

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

SEMESTER-II

Course Code: CHEMISTRY –Core Paper-2

Course Title: Chemical Energetics, Equilibria and Functional Group Organic Chemistry-I

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

Section A: Physical Chemistry (Lectures:30)

Unit 1:

Chemical Energetics

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

(Lectures: 8)

Unit 2:

Chemical Equilibrium

Free energy change in a chemical reaction, Thermodynamic derivation of the law of chemical equilibrium, distinction between G and G_0 , Le Chatelier's principle, relationships between K_p , K_c and K_x for reactions involving ideal gases.

(Lectures: 8)

Unit 3:

Ionic Equilibria

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

(Lectures: 14)

Section B: Organic Chemistry (Lectures: 30)

Unit 4:

Aromatic Hydrocarbons

Structure and aromatic character of benzene.

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

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

(Lectures: 5)

Unit 5:

Alkyl and Aryl Halides

A) Alkyl halides (upto 5 carbons):

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

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

Reactions: Nucleophilic substitution reactions with mechanism and their types (S_N1 , S_N2 and S_Ni), competition with elimination reactions (elimination vs substitution), nucleophilic substitution reactions with

specific examples from: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation and Williamson's ether synthesis.

B) Haloarenes:

Structure and resonance

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

Reaction: Nucleophilic aromatic substitution by OH group (Bimolecular Displacement Mechanism), Effect of nitro substituent on reactivity of haloarenes, Reaction with strong bases $\text{NaNH}_2/\text{NH}_3$ (elimination-addition mechanism involving benzyne intermediate), relative reactivity and strength of C-X bond in alkyl, allyl, benzyl, vinyl and aryl halides.

(Lectures:11)

Unit 6:

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

A) Alcohols (upto 5 Carbon):

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

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

Reactions: Acidic character of alcohols and reaction with sodium, with HX (Lucas Test), esterification, oxidation (with PCC, alkaline KMnO_4 , acidic $\text{K}_2\text{Cr}_2\text{O}_7$ 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 , $\text{NH}_2\text{-G}$ derivatives. Iodoform test, Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemmensen reduction, Wolff Kishner reduction, Meerwein-Ponndorf Verley reduction.

Practical:

(Credits: 2, Laboratory periods: 60)

Section A: Physical Chemistry

Energetics:

1. Determination of heat capacity of calorimeter.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of integral enthalpy of solution of salts (KNO_3 , NH_4Cl).
4. Determination of enthalpy of hydration of copper sulphate.

Ionic equilibria:

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

Section B: Organic Chemistry

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

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

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

References:

Theory:

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

7. Bahl, A; Bahl, B. S. (2012), **Advanced Organic Chemistry**, S. Chand.

Practical:

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

Additional Resources:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

SEMESTER –III

Course Code: CHEMISTRY –Core Paper-3

Course Title: Solutions, Phase Equilibrium, Conductance, Electrochemistry and Functional Group Organic Chemistry-II

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

The students will learn about ideal and non-ideal solutions, Raoult's law, partially miscible and immiscible solutions and their applications. The student will also learn about equilibrium between phases with

emphasis on one component and simple eutectic systems. In electrochemical cells the students will learn about electrolytic and galvanic cells, measurement of conductance and its applications, measurement of emf and its applications. The topics of carbohydrates, amino acids, peptides and proteins are introduced through some specific examples. A relationship between structure, reactivity and biological properties of biomolecules is established through the study of these representative biomolecules.

Learning Outcomes:

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

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

Section A: Physical Chemistry (Lectures:30)

Unit 1:

Solutions

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

(Lectures: 6)

Unit 2:

Phase Equilibrium

Phases, components and degrees of freedom of a system, criteria of phase equilibrium, Gibbs phase rule and its thermodynamic derivation, derivation of Clausius- Clapeyron equation and its importance in phase equilibria, phase diagrams of one component systems (water and sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver, $\text{FeCl}_3\text{-H}_2\text{O}$ and Na-K only).

(Lectures: 6)

Unit 3:

Conductance

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

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

(Lectures: 8)

Unit 4:

Electrochemistry

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

(Lectures: 10)

Section B: Organic Chemistry (Lectures:30)

Unit 5:

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

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

Preparation: Acidic and alkaline hydrolysis of esters.

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

Carboxylic acid derivatives (aliphatic):

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

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

B) Amines (aliphatic & aromatic) and Diazonium Salts

Amines

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

Reactions: Hofmann vs Saytzeff elimination, carbylamine test, Hinsberg test, reaction with HNO_2 , Schotten-Baumann reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation, basicity of amines.

Diazonium salt

Preparation: from aromatic amines

Reactions: conversion to benzene, phenol and dyes.

(Lectures: 13)

Unit 6:

Amino Acids, Peptides and Proteins

Zwitterion, isoelectric point and electrophoresis

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

Reactions of amino acids: ester of $-\text{COOH}$ group, acetylation of $-\text{NH}_2$ group, complexation with Cu^{2+} ions, ninhydrin test.

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

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

(Lectures: 9)

B) Carbohydrates

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

(Lectures:8)

Practical:

(Credits: 2, Laboratory periods: 60)

Section A: Physical Chemistry

Phase Equilibria

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

Conductance

1. Determination of cell constant.
2. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
3. Perform the following conductometric titrations:

a) Strong acid vs strong base

b) Weak acid vs strong base.

Potentiometry

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

Section B: Organic Chemistry

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

References:

Theory:

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

Practical:

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), **Senior Practical Physical Chemistry**, R. Chand & Co.

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

SEMESTER-IV

Course Code: CHEMISTRY –Core Paper-4

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

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

Section A: Inorganic Chemistry (Lectures:30)

Unit 1:

General Principles of Metallurgy

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

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

(Lectures: 4)

Unit 2:

s- and p- block elements

Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electronegativity (Pauling, Mulliken, and Allred-Rochow scales). Allotropy in C, S, and P. Oxidation states with reference to elements in unusual and rare oxidation states like carbides and nitrides), inert pair effect, diagonal relationship and anomalous behaviour of first member of each group. ,compounds of s- and p-block elements , diborane and concept of multicentre bonding. Structure, bonding and their important properties like oxidation/reduction, acidic/basic nature of the following compounds and their applications in industrial and environmental chemistry. Hydrides of nitrogen (NH_3 , N_2H_4 , N_3H , NH_2OH) Oxoacids of P, S and Cl, Halides and oxohalides: PCl_3 , PCl_5 , SOCl_2 and SO_2Cl_2 .

(Lectures: 26)

Section B: Physical Chemistry (Lectures:30)

Unit 3:

Kinetic Theory of Gases

Postulates of kinetic theory of gases and derivation of the kinetic gas equation, deviation of real gases from ideal behaviour, compressibility factor, causes of deviation, van der Waals equation of state for real gases. Boyle temperature (derivation not required), critical phenomena, critical constants and their calculation from van der Waals equation, Andrews isotherms of CO_2 , Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance. Temperature dependence of these distributions, most probable, average and root mean square velocities (no derivation), collision cross section, collision number, collision frequency, collision diameter and mean free path of molecules, viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only).

(Lectures: 10)

Unit 4:

Liquids

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

(Lectures: 3)

Unit 5:

Solids

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

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

(Lectures: 6)

Unit 6:

Chemical Kinetics

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

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

(Lectures: 11)

Practical:

(Credits: 2, Laboratory periods: 60)

Section A: Inorganic Chemistry

Semi-micro qualitative analysis of mixtures using H₂S or any other scheme- not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations: NH₄⁺, Pb²⁺, Bi³⁺, Cu²⁺, Cd²⁺, Fe³⁺, Al³⁺, Co²⁺, Ni²⁺, Mn²⁺, Zn²⁺, Ba²⁺, Sr²⁺, Ca²⁺, K⁺

Anions: CO₃²⁻, S²⁻, SO₃⁻, NO₂⁻, CH₃COO⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, SO₄²⁻, PO₄³⁻, BO₃³⁻, C₂O₄²⁻, F⁻.

(Spot tests should be carried out wherever feasible)

Section B: Physical Chemistry

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

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

2. Viscosity measurement (use of organic solvents excluded):

- Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald viscometer.
- Study of the variation of viscosity of an aqueous solution with concentration of solute.

3. Chemical Kinetics

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

- Acid hydrolysis of methyl acetate with hydrochloric acid.
- Compare the strength of HCl and H₂SO₄ by studying the kinetics of hydrolysis methyl acetate.

References:

Theory:

- Lee., J. D. **A new Concise Inorganic Chemistry**, Pearson Education.

2. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), **Shriver and Atkin's Inorganic Chemistry**, Oxford.
3. Miessler, G. L.; Tarr, D.A.(2014), **Inorganic Chemistry**, Pearson.
4. Castellan, G. W.(2004), **Physical Chemistry**, Narosa.
5. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol.1, 6th Edition, McGraw Hill Education.
6. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol.5, 3rd Edition, McGraw Hill Education.
7. B.R.Puri, L.R.Sharma, M.S.Pathania, (2017), **Principles of Physical Chemistry**, Vishal Publishing Co.

Practical:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

CHEMISTRY DISCIPLINE ELECTIVE COURSES (DSE)

Chemistry of d block elements, Quantum Chemistry and Spectroscopy is compulsory.
Choose any one more.

Course Code: CHEMISTRY –DSE-1

Course Title: Applications of Computers in Chemistry

Total Credits: 06

(Credits: Theory-04, Practicals-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Basic Computer system (in brief)

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

(Lectures: 5)

Unit 2:

Use of Programming Language for solving problems in Chemistry

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

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

Simple programs using above mentioned commands.

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

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

(Lectures: 40)

Unit 3:

Use of Software Products

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

(Lectures: 15)

Practical:

(Credits: 2, Laboratory periods: 60)

Computer programs using QBASIC based on numerical methods

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

Use of Software Products

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

References:

Theory:

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

Practical:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-2

Course Title: Analytical Methods in Chemistry

Total Credits: 06

(Credits: Theory-04, Practicals-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Qualitative and quantitative aspects of analysis:

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

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

(Lectures: 5)

Unit 2:

Optical methods of analysis

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

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

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

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

(Lectures: 25)

Unit 3:

Thermal methods of analysis:

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

(Lectures: 5)

Unit 4:

Electroanalytical methods

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

(Lectures:10)

Unit 5:

Separation techniques

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

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

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

(Lectures:15)

Practical:

(Credits: 2, Laboratory periods: 60)

1. Separation of mixtures by paper chromatography and reporting the R_f values:
 - (i) Co^{2+} and Ni^{2+} .
 - (ii) Amino acids present in the given mixture.
2. 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.
3. Analysis of soil:
- (i) Determination of pH of soil.
(ii) Total soluble salt
(iii) Estimation of calcium and magnesium
(iv) Qualitative detection of nitrate and phosphate
4. Ion exchange:
- (i) Determination of exchange capacity of cation exchange resins and anion exchange resins.
(ii) Separation of amino acids from organic acids by ion exchange chromatography.
5. Spectrophotometry
- (i) Verification of Lambert-Beer's law and determination of concentration of a coloured species (CuSO_4 , KMnO_4 , CoCl_2 , CoSO_4)
(ii) Determination of concentration of coloured species via following methods;
1. Graphical method, (b) Epsilon method, (c) Ratio method, (iv) Standard addition method

References:

Theory:

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

Practical:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-3

Course Title: Molecular Modelling and Drug Design

Total Credits: 06

(Credits: Theory-04, Practicals-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

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

Coordinate systems: Cartesian and Internal Coordinates, Bond lengths, bond angles and torsion angles, Writing Z -matrix (ex: methane, ethane, ethene, ethyne, water, H₂O₂ .

(Lectures: 8)

Unit 2:

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

Applications of computational chemistry to determine reaction mechanisms.

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

(Lectures: 12)

Unit 3:

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

(Lectures: 10)

Unit 4:

Molecular Dynamics: Radial distribution functions for solids, liquids and gases, intermolecular Potentials (Hard sphere, finite square well and Lennard-Jones potential), concept of periodic box, ensembles (microcanonical, canonical, isothermal – isobaric), Ergodic hypothesis. Integration of Newton's equations (Leapfrog and Verlet Algorithms), Rescaling, Simulation of Pure water – Radial distribution curves and interpretation, TIP & TIP3P, Typical MD simulation

Brief introduction to Langevin and Brownian dynamics

Monte Carlo Method: Metropolis algorithm.

(Lectures: 10)

Unit 5:

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

Extension to Extended Huckel theory and PPP methods

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

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

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

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

(Lectures: 12)

Unit 6:

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

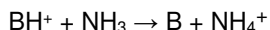
QSAR: Structure-activity relationships. Properties in QSAR (Partial atomic charges, polarizabilities, volume and surface area, log P, lipophilicity and Hammett equation and applications, hydration energies, refractivity). Biological activities (LD50, IC50, ED50.)

(Lectures: 8)

Practical:

(Credits: 2, Laboratory periods: 60)

1. Plotting a 3D graph depicting a saddle point in a spreadsheet software.
2. Determine the enthalpy of isomerization of cis and trans 2-butene.
3. Determine the heat of hydrogenation of ethylene.
4. Compare the optimized C-C bond lengths and Wiberg bond orders in ethane, ethene, ethyne and benzene using PM3. Is there any relationship between the bond lengths and bond orders? Visualize the highest occupied and lowest unoccupied molecular orbitals of ethane, ethene, ethyne, benzene and pyridine.
5. Perform a conformational analysis of butane.
6. Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine by comparison of their Mulliken charges and ESP maps.
7. Compare the gas phase basicities of the methylamines by comparing the enthalpies of the following reactions:

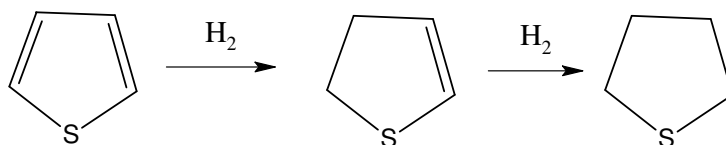


where B = CH₃NH₂, (CH₃)₂NH, (CH₃)₃N

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 H₂O, H₂S, H₂Se using PM3.
10. Compare the HAH bond angles for the second row hydrides (BeH₂, CH₄, NH₃, H₂O) and compare with the results from qualitative MO theory.
11. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
12. Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
13. Plot the electrostatic potential mapped on electron density for benzene and use it to predict the type of stacking in the crystal structure of benzene dimer.
14. Predict the aromaticity of thiophene with respect to benzene by comparing the enthalpies of the following reactions:

(a) Hydrogenation of benzene to 1,3-cyclohexadiene and then 1,3-cyclohexadiene to cyclohexene.

(b)



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

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

References:

Theory:

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

Practical:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-4

Course Title: Novel Inorganic Solids

Total Credits: 06

(Credits: Theory-04, Practicals-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

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

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

(Lectures: 10)

Unit 2:

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

(Lectures: 10)

Unit 3:

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

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

(Lectures: 10)

Unit 4:

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

(Lectures: 10)

Unit 5:

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

(Lectures: 10)

Unit 6:

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

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

(Lectures: 10)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Practical: Novel Inorganic Solids

1. Synthesis of silver nanoparticles by chemical methods and characterization using UV-visible spectrophotometer.
2. Synthesis of silver nanoparticles by green approach methods and characterization using UV-visible spectrophotometer.
3. Preparation of polyaniline and its characterization using UV-visible spectrophotometer.

4. Synthesis of metal sulphide nanoparticles (MnS, CdS, ZnS, CuS, NiO) and characterization using UV-visible spectrophotometer.
5. Intercalation of hydrogen in tungsten trioxide and its conductivity measurement using conductometer.
6. Synthesis of inorganic pigments (PbCrO₄, ZnCrO₄, Prussian Blue, Malachite).
7. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.
8. Preparation of zeolite A and removal of Mg and Ca ions from water samples quantitatively using zeolite.

References:

Theory:

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

Practicals:

1. Orbaek, W.; McHale, M.M.; Barron, A. R.; **Synthesis and Characterization of Silver Nanoparticles for An Undergraduate Laboratory**, J. Chem. Educ. 2015, 92, 339–344.
2. MacDiarmid, G.; Chiang, J.C.; Richter, A.F.; Somasiri, N.L.D.(1987), **Polyaniline: Synthesis and Characterization of the Emeraldine Oxidation State by Elemental Analysis**, L. Alcaeer (ed.), *Conducting Polymers*, 105-120, D. Reidel Publishing.
3. Cheng, K.H.; Jacobson, A.J.; Whittingham, M.S. (1981), **Hexagonal Tungsten Trioxide and Its Intercalation Chemistry**, *Solid State Ionics*, 5, 1981, 355-358.
4. Ghorbani H.R.; Mehr, F.P; Pazoki, H; Rahmani, B.M.; **Synthesis of ZnO Nanoparticles by Precipitation Method**, *Orient J Chem* 2015, 31(2).

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-5

Course Title: Polymer Chemistry

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

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

Unit 1:

Introduction and history of polymeric materials:

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

Functionality and its importance:

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

(Lectures: 12)

Unit 2:

Kinetics of Polymerization

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

(Lectures: 8)

Unit 3:

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

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

Nature and structure of polymers-Structure Property relationships

(Lectures: 14)

Unit 4:

Determination of molecular weight of polymers (M_n , M_w , etc.) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index

Polymer Solution

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

Polymer Degradation

Thermal, oxidative, hydrolytic and photodegradation

(Lectures: 16)

Unit 5:

Properties of Polymers

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

(Lectures: 10)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Polymer chemistry

Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA)/MethylAcrylate (MA).

2. Preparation of nylon 6,6
3. Redox polymerization of acrylamide
4. Precipitation polymerization of acrylonitrile
5. Preparation of urea-formaldehyde resin
6. Preparations of novalac resin/resold resin.
7. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

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

Polymer analysis

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

Suggested Additional Experiment:

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

References:

Theory:

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

Practical:

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

Teaching-Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-6

Course Title: Research Methodology For Chemistry

Total Credits: 06

(Credits: Theory-05, Tutorial-01)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Literature Survey

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

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

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

(Lectures: 20)

Unit 2:

Methods of Scientific Research and Writing Scientific Papers

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

(Lectures: 20)

Unit 3:

Chemical Safety and Ethical Handling of Chemicals

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

(Lectures: 12)

Unit 4:

Data Analysis

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

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

Biostatistics: brief introduction and data handling.

(Lectures: 13)

Exposure of chemistry software

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

(Lectures: 10)

References:

Theory:

1. Dean, J.R.; Jones, A.M.; Holmes, D.; Reed, R.; Jones, A.Weyers, J. (2011), **Practical skills in chemistry**, Prentice-Hall.
2. Hibbert, D.B.; Gooding, J.J. (2006), **Data analysis for chemistry**, Oxford University Press.
3. Topping, J.(1984), **Errors of observation and their treatment**, Chapman Hall, London.
4. Levie, R. de.(2001), **How to use Excel in analytical chemistry and in general scientific data analysis**, Cambridge University Press.
5. Le, C.T.; Eberly, L.E. (2016), **Introductory Biostatistics**, Wiley.

Additional References:

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

Teaching Learning Process

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

Assessment Methods

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

Keywords

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

Course Code: CHEMISTRY –DSE-7

Course Title: Green Chemistry

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

Today's society is moving towards becoming more and more environmentally conscious. There is rising concern of environmental pollution, depleting resources, climate change, ozone depletion, heaps and heaps of landfills piling up, legislation which is getting stringent with strict environmental laws, rising cost of waste deposits and so on. We are faced with a challenge to work towards sustainable practices. Green chemistry has arisen from these concerns. It is not a new branch of chemistry but the way chemistry should be practiced.

Innovations and applications of green chemistry in education has helped companies not only gain environmental benefits but at the same time achieve economic and societal goals also. This is possible because these undergraduate students are ultimate scientific community of tomorrow.

Learning Outcomes:

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

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

Unit 1:

Introduction to Green Chemistry

What is Green Chemistry? Some important environmental laws, pollution prevention Act of 1990, emergence of green chemistry, Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

(Lectures:5)

Unit 2:

Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry and their explanation with examples

Special emphasis on the following:

- Prevention of Waste/ by products; maximum incorporation of the materials used in the process into the final products, Environmental impact factor, waste or pollution prevention hierarchy
- Green metrics to assess greenness of a reaction, e.g. Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
- Prevention/ minimization of hazardous/ toxic products reducing toxicity
- Risk = (function) hazard x exposure
- Designing safer chemicals with minimum toxicity yet has the ability to perform the desired functions
- Green solvents: super critical fluids with special reference to carbon dioxide, water as a solvent for organic reactions, ionic liquids, fluorinated biphasic solvent, PEG, solventless processes, solvents obtained from renewable resources and how to compare greenness of solvents
- Energy requirements for reactions – alternative sources of energy: use of microwaves, ultrasonic energy and photochemical energy

- Selection of starting materials; should be renewable rather than depleting, Illustrate with few examples such as biodiesel and polymers from renewable resources (such as green plastic)
- Avoidance of unnecessary derivatization – careful use of blocking/protecting groups
- Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
- Design for degradation: A product should not persist after the commercial function is over e.g. soaps and detergents, pesticides and polymers
- Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.
- Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD “What you don’t have cannot harm you”, greener alternative to Bhopal Gas Tragedy (safer route to carbonyl) and Flixborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.

(Lectures:25)

Unit 3:

Examples of Green Synthesis/ Reactions

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

(Lectures:1

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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 CO₂ for precision cleaning and dry cleaning of garments.
- A new generation of environmentally advanced wood preservatives: Getting the chromium and Arsenic out of pressure treated wood.
- An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn.
- Healthier Fats and oils by Green Chemistry: Enzymatic Inter esterification for production of No Trans-Fats and Oils.
- Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting.
- Using a naturally occurring protein to stimulate plant growth, improve crop quality, increase yields, and suppress disease.

(Lectures:10)

Unit 5:

Future Trends in Green Chemistry

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

(Lectures:10)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab- Green chemistry

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

Safer starting materials

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

Using renewable resources

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

Use of enzymes as catalysts

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

Alternative green solvents

4. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.
5. Mechanochemical solvent free, solid–solid synthesis of azomethine using p- toluidine and o-vanillin/p-vanillin (various other combinations of primary amine and aldehyde can also be tried).

Alternative sources of energy

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

Reducing waste

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

Some representative examples:

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

References:

Theory:

1. Anastas, P.T.; Warner, J.C.(1998), **Green Chemistry, Theory and Practice**, Oxford University Press.

2. Lancaster, M.(2016),**Green Chemistry An Introductory Text**.2nd Edition, RSC Publishing.
3. Cann , M. C.; Umile, T.P. (2008), **Real world cases in Green chemistry** Vol 11, American chemical Society,Washington.
4. Matlack, A.S.(2001),**Introduction to Green Chemistry**, Marcel Dekker.
5. Alhuwalia, V. K.; Kidwai, M.R.(2005),**New Trends in Green chemistry**, Anamalaya Publishers.

Practical:

1. Kirchoff, M.; Ryan, M.A. (2002), **Greener approaches to undergraduate chemistry experiment**. American Chemical Society, Washington DC.
2. Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K.(2013), **Green Chemistry Experiments: A monograph**, I.K. International Publishing House Pvt Ltd. New Delhi.
3. Pavia,D.L.; Lamponam, G.H.; Kriz, G.S.W. B.(2006),**Introduction to organic Laboratory Technique- A Microscale approach**,4th Edition, Brrooks-Cole Laboratory Series for Organic chemistry.
4. Wealth from Waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated. Indu Tucker Sidhwani et al. University of Delhi, Journal of Undergraduate Research and Innovation, Volume 1, Issue 1,February 2015, ISSN: 2395-2334.
5. Sidhwani, Tucker I.; Chowdhury, S. Greener alternatives to Qualitative Analysis for Cations without H₂S and other sulfur containing compounds, J. Chem. Educ. 2008, 85, 1099.
6. Sidhwani, Tucker I.; Chowdhury, S. et al., DU Journal of Undergraduate Research and Innovation2016, Volume 2, Issue 2, 70-79.
7. Dhingra, S., ;Angrish, C. Qualitative organic analysis: An efficient, safer, and economical approach to preliminary tests and functional group analysis. *Journal of Chemical Education*, 2011, 88(5), 649-651.

Teaching Learning Process:

- Conventional chalk and board teaching
- Power point presentations
- Interactive sessions
- Literature survey and critical thinking to design to improve a traditional reaction and problem solving
- Visit to a green chemistry lab
- Some motivating short movies in green chemistry especially in bio mimicry

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-8

Course Title: Industrial Chemicals and Environment

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Industrial Gases: Large scale production, uses storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, and sulphur dioxide.

(Lectures: 6)

Unit 2:

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

(Lectures: 10)

Unit 3:

Industrial Metallurgy: Preparation of ultrapure metals for semiconductor technology.

(Lectures: 4)

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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 SO₂, CO₂, CO, NO_x, H₂S and other foul smelling gases, methods of estimation of CO, NO_x, SO_x and control procedures, Effects of air pollution on living organisms and vegetation

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

(Lectures:15)

Unit 5:

Water Pollution:

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

Sludge disposal. Industrial waste management, incineration of waste.

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

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

(Lectures:15)

Unit 6:

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

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

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

(Lectures: 10)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Industrial Chemicals & Environment

1. Determination of dissolved oxygen in water.
2. Determination of Chemical Oxygen Demand (COD).
3. Determination of Biological Oxygen Demand (BOD).
4. Percentage of available chlorine in bleaching powder.
5. Measurement of chloride, sulphate and salinity of water samples by simple titration method (AgNO₃ and potassium chromate).
6. Estimation of total alkalinity of water samples (CO₃²⁻, HCO₃⁻) using double titration method.
7. Measurement of dissolved CO₂
8. Determination of hexavalent Chromium Cr(VI) concentration in tannery wastes/waste water sample using UV-Vis spectrophotometry technique.
9. Preparation of borax/ boric acid

References:

Theory

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

Practical

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-9

Course Title: Inorganic Materials of Industrial Importance

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 able to:

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

Unit 1:

Silicate Industries

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

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

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

(Lectures: 10)

Unit 2:

Fertilizers:

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

(Lectures: 10)

Unit 3:

Surface Coatings:

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

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

(Lectures: 18)

Unit 4:

Batteries:

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

(Lectures: 8)

Unit 5:

Engineering materials for mechanical construction:

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

(Lectures: 8)

Unit 6:

Nano dimensional materials

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

(Lectures: 6)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Inorganic materials of industrial importance

1. Detection of constituents of Ammonium Sulphate fertilizer (Ammonium and Sulphate ions) by qualitative analysis and determine its free acidity.
2. Detection of constituents of CAN fertilizer (Calcium, Ammonium and Nitrate ions) fertilizer and estimation of Calcium content.
3. Detection of constituents of Superphosphate fertilizer (Calcium and Phosphate ions) and estimation of phosphoric acid content.
4. Detection of constituents of Dolomite (Calcium, Magnesium and carbonate ions) and determination of composition of Dolomite (Complexometric titration).
5. Analysis of (Cu, Ni) in alloy or synthetic samples (Multiple methods involving Complexometry, Gravimetry and Spectrophotometry).
6. Analysis of (Cu, Zn) in alloy or synthetic samples (Multiple methods involving Iodometry, Complexometry and Potentiometry).
7. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.
8. Synthesis of silver nanoparticles by green and chemical approach methods and its characterization using UV-visible spectrophotometer.

References:

Theory:

1. West, A. R. (2014), **Solid State Chemistry and Its Application**, Wiley
2. Smart, L. E.; Moore, E. A. (2012), **Solid State Chemistry An Introduction**, CRC Press Taylor & Francis.
3. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A.(2010), **Shriver and Atkins Inorganic Chemistry**, W. H. Freeman and Company.
4. Kent, J. A. (ed) (1997), **Riegel's Handbook of Industrial Chemistry**, CBS Publishers, New Delhi.
5. Poole Jr.; Charles P.; Owens, Frank J.(2003), **Introduction to Nanotechnology**, John Wiley and Sons.

Practical:

1. Svehla, G.(1996), **Vogel's Qualitative Inorganic Analysis**, Prentice Hall.
2. Banewicz, J. J.; Kenner, C.T. **Determination of Calcium and Magnesium in Limestones and Dolomites**, Anal. Chem., 1952, 24 (7), 1186–1187.
3. Ghorbani, H. R.; Mehr, F.P.; Pazoki, H.; Rahmani B. M. **Synthesis of ZnO Nanoparticles by Precipitation Method**. Orient J Chem 2015;31(2).
4. Orbaek, W.; McHale, M.M.; Barron, A.R. **Synthesis and characterization of silver nanoparticles for an undergraduate laboratory**, J. Chem. Educ. 2015, 92, 339–344.

Additional Resources:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-10

Course Title: Instrumental Methods of Chemical Analysis

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

This course aims to provide knowledge on various spectroscopic techniques for chemical analysis along with the basic principles of instrumentation.

Learning Outcomes:

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

- Handle analytical data
- Understand basic components of IR, FTIR, UV-Visible and Mass spectrometer.
- Interpret of IR, FTIR, UV-visible spectra and their applications.
- Understand the use of single and double beam instruments.
- Learn separations techniques like Chromatography.
- Learn 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.

(Lectures: 4)

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.

(Lectures: 8)

Unit 3:

UV-Visible/ Near IR Spectroscopy

Emission, absorption, fluorescence and photoacoustic. 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, photoacoustic, fluorescent tags).

(Lectures: 8)

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.

(Lectures: 8)

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.

(Lectures: 8)

Unit 6:

Elemental analysis

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Mass spectrometry (electrical discharges).

Atomic spectroscopy: Atomic absorption, atomic emission, and atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), wavelength 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).

(Lectures: 8)

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

(Lectures:

4)

Electroanalytical Methods: Potentiometry & Voltammetry. **(Lectures: 4)**

Radiochemical Methods. **(Lectures: 4)**

X-ray analysis and electron spectroscopy (surface analysis). **(Lectures: 4)**

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Instrumental methods of chemical analysis

At least 10 experiments to be performed.

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 absorption spectroscopy.
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.

References:

Theory:

1. Willard, H.H.; Merritt, L.L. Jr.; Dean, J.A.; Settle, F.A. Jr.(2004), **Instrumental methods of analysis**, 7th edition, CBS Publishers.
2. Christian, G.D.(2004), **Analytical Chemistry**, 6th Edition, John Wiley & Sons, New York.
3. Skoog, D.A.; Holler, F. J.; Crouch, S.(2006), **Principles of Instrumental Analysis**, Thomson Brooks/Cole.
4. Banwell, C.N. (2006), **Fundamentals of Molecular Spectroscopy**, Tata McGraw-Hill Education

Practical:

1. Skoog, D. A.; Holler, F. J.; Crouch, S.(2006), **Principles of Instrumental Analysis**, Cengage Learning.
2. Willard, H.H.; Merritt, L.L. Jr.; Dean, J.A.; Settle, F.A. Jr.(2004), **Instrumental methods of analysis**, 7th edition, CBS Publishers.

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

Analytical 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, Electronic spectroscopy.

Course Code: CHEMISTRY –DSE-11

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

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

Section A: Inorganic Chemistry (Lectures:30)

Unit 1:

Transition Elements (3d series)

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

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

(Lectures: 10)

Unit 2:

Coordination Chemistry

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

(Lectures: 6)

Unit 3:

Bonding in coordination compounds

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

Crystal Field Theory

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

(Lectures: 14)

Section B: Physical Chemistry (Lectures:30)

Unit 4:

Quantum Chemistry

Postulates of quantum mechanics, quantum mechanical operators.

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

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

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

(Lectures: 12)

Unit 5:

Spectroscopy

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

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

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

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

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

(Lectures: 12)

Unit 6:

Photochemistry

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

(Lectures: 6)

Practical:

(Credits: 2, Laboratory periods: 60)

Section A: Inorganic Chemistry

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

Section B: Physical Chemistry

UV/Visible spectroscopy

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 ($J\ molecule^{-1}$, $kJ\ mol^{-1}$, 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.

Colorimetry

1. Verify Lambert-Beer's law and determine the concentration of $CuSO_4/KMnO_4/K_2Cr_2O_7/CoSO_4$ in a solution of unknown concentration

Chemical Kinetics; Study the kinetics of the following reactions.

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

References:

Theory:

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

7. B.R.Puri, L.R.Sharma, M.S.Pathania, (2017), **Principles of Physical Chemistry**, Vishal Publishing Co.

Practical:

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

Additional Resources:

1. Castellan, G. W.(2004), **Physical Chemistry**, Narosa.
2. Petrucci, R. H.(1989), **General Chemistry: Principles and Applications**, Macmillan Publishing Co.

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-12

Course Title: Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons and UV, IR Spectroscopy

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

The purpose of the course is to introduce students to some important 3d metals and their compounds which they are likely to come across. Students learn about organometallic compounds and bioinorganic chemistry which are currently frontier areas of chemistry providing an interface between organic chemistry, inorganic Chemistry and biology. The functional group approach to organic chemistry

introduced in the previous courses is reinforced through the study of the chemistry of carboxylic acids and their derivatives, Amines and diazonium salts, active methylene compounds. The students will also be introduced to the chemistry and applications of polynuclear hydrocarbons and heterocyclic compounds. The learners are introduced to spectroscopy, an important analytical tool which allows identification of organic compounds by correlating their spectra to structure.

Learning Outcomes:

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

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

Section A: Inorganic Chemistry (Lectures:30)

Unit 1:

Chemistry of 3d metals

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

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

$\text{K}_2\text{Cr}_2\text{O}_7$, KMnO_4 , $\text{K}_4[\text{Fe}(\text{CN})_6]$.

(Lectures: 6)

Unit 2:

Organometallic Compounds

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

(Lectures: 12)

Unit 3:

Bio-Inorganic Chemistry

A brief introduction to bio-inorganic chemistry. Role of metal ions present in biological systems with special reference to Na⁺, K⁺ and Mg²⁺ ions: Na/K pump; Role of Mg²⁺ ions in energy production and chlorophyll. Brief introduction to oxygen transport and storage (haemoglobin-myoglobin system). Brief introduction about toxicity of metal ions (Hg²⁺ and Cd²⁺).

(Lectures: 12)

Section B: Organic Chemistry (Lectures:30)

Unit 4:

Polynuclear and heteronuclear aromatic compounds:

Structure elucidation of naphthalene, preparation and properties of naphthalene and anthracene.

Preparation and Properties of the following compounds with reference to electrophilic and nucleophilic substitution: furan, pyrrole, thiophene, and pyridine.

(Lectures: 13)

Unit 5:

Active methylene compounds

Preparation: Claisen ester condensation, Keto-enol tautomerism.

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

(Lectures: 5)

Unit 6:

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

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

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

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

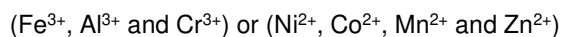
(Lectures: 12)

Practical:

(Credits: 2, Laboratory periods: 60)

Section A: Inorganic Chemistry

1. Separation of mixtures of two ions by paper chromatography and measurement of R_f value in each case:



2. Preparation of any two of the following complexes and measurement of their conductivity:

(i) tetraamminecopper (II) sulphate (ii) potassium trioxalatoferrate (III) trihydrate.

Compare the conductance of the complexes with that of M/1000 solution of NaCl, MgCl₂ and LiCl₃.

Section B: Organic Chemistry

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

References:

Theory:

1. Huheey, J.E.; Keiter, E.A.; Keiter, R. L.; Medhi, O.K. (2009), **Inorganic Chemistry- Principles of Structure and Reactivity**, Pearson Education.
2. Lee, J. D. **A new Concise Inorganic Chemistry**, Pearson Education.
3. Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994), **Concepts and Models of Inorganic Chemistry**, John Wiley & Sons.
4. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), **Shriver and Atkins Inorganic Chemistry**, 5th Edn, W. H. Freeman and Company, 41 Madison Avenue, New York, NY.
5. Finar, I. L. **Organic Chemistry** (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
6. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
7. Bahl, A; Bahl, B. S. (2012), **Advanced Organic Chemistry**, S. Chand.

Practical:

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

Additional Resources:

1. Cotton, F. A.; Wilkinson, G.; Gaus, P.L. (1995), **Basic Inorganic Chemistry**, 3rd Edition, John Wiley.
2. Sharpe, A.G.(2005), **Inorganic Chemistry**, Pearson Education.
3. Greenwood, N.N.; Earnshaw, A.(1997), **Chemistry of the Elements**, Elsevier.
4. Silverstein, R.M.; Bassler, G.C.; Morrill, T.C. (1991), **Spectroscopic Identification of Organic Compounds**, John Wiley & Sons.

5. Dyer, J.R.(1978), **Applications of Absorption Spectroscopy of Organic Compounds**, Prentice Hall.

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-13

Course Title: Molecules of Life

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Carbohydrates

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

(Lectures: 10)

Unit 2:

Amino Acids, Peptides and Proteins

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

(Lectures: 12)

Unit 3:

Enzymes and correlation with drug action

Classification of enzymes and their uses (mention Ribozymes). Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (Competitive and non-competitive inhibition including allosteric inhibition). Drug action-receptor theory. Structure – activity relationships of drug molecules, binding role of –OH group, –NH₂ group, double bond and aromatic ring.

(Lectures: 10)

Unit 4:

Nucleic Acids

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

(Lectures: 10)

Unit 5:

Lipids

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

(Lectures: 8)

Unit 6:

Concept of Energy in Biosystems

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

(Lectures: 10)

Practical:

(Credits: 2, Laboratory periods: 60)

1. Separation of amino acids by paper chromatography
2. Study of titration curve of glycine and determination of its isoelectric point.
3. Estimation of proteins by Lowry's method
4. Action of salivary amylase on starch
5. Effect of temperature on the action of salivary amylase on starch.
6. To determine the saponification value of an oil/fat.
7. To determine the iodine value of an oil/fat
8. Qualitative tests for carbohydrates- Molisch test Barfoed's reagent test, rapid furfural test, Tollen's test and Fehling solution test(Only these tests are to be done in class)
9. Qualitative tests for proteins
10. Extraction of DNA from onion/cauliflower

References:

Theory:

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

Practical:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –DSE-14

Course Title: Nanoscale Materials and Their Applications

Total Credits: 06

(Credits: Theory-04, Practical-02)

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

Objectives:

The aim of this course is to introduce materials at nanoscale, their preparation, characterization and applications.

Learning Outcomes:

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

- Understand the concept of nanodimensions.
- Know the various methods of preparation of nanomaterials.
- Know the different characterization techniques used for the analysis of nanomaterials and understand the basic principle behind these techniques.

- Understand the optical and conducting properties of nanostructures.
- Appreciate the real life applications of nanomaterials.

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.

(Lectures: 10)

Unit 2:

Preparation of nanomaterials

Top down and Bottom up approach, Photolithography. Ball milling. Vacuum deposition. Physical vapor deposition (PVD), Chemical vapor deposition (CVD), Thermal decomposition, Chemical reduction, Sol-Gel synthesis, Hydrothermal synthesis, Spray pyrolysis, Electrochemical deposition, Pulsed Laser deposition.

(Lectures: 8)

Unit 3:

Characterization techniques (*Basic working principles and interpretation of experimental data using these techniques need to be covered*)

UV-visible spectroscopy, X-ray diffraction (Powder and Single Crystal), Raman Spectroscopy, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Energy Dispersive X-ray Spectroscopy (EDX), X-ray Photoelectron Spectroscopy (XPS), Atomic Force Microscopy (AFM), Scanning Tunneling Microscopy (STM), Dynamic light scattering (DLS), Brunauer-Emmett-Teller (BET) Surface area measurement and Thermogravimetric analysis (TG).

(Lectures: 14)

Unit 4:

Optical Properties

Surface plasmon resonance, Excitons in direct and indirect band gap semiconductor nanocrystals. Radiative processes: General absorption, emission and luminescence (fluorescence and photoluminescence). (Lectures: 8)

Unit 5:

Conducting properties

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

Unit 6:

Applications

Nanomaterials as Catalysts, semiconductor nanomaterials as photocatalysts, nanocomposites as catalysts.

Carbon nanostructures as catalytic nanoreactors, metal and metal oxides confined inside carbon nanostructures, Nanowires and thin films for photonic devices (LEDs, solar cells, transistors).

(Lectures:14)

References:

1. West, A. R.(2014),**Solid State Chemistry and Its Application**, Wiley
2. Smart, L. E.; Moore, E. A.(2012),**Solid State Chemistry An Introduction**, CRC Press Taylor & Francis.
3. Rao, C. N. R.; Gopalakrishnan, J.(1997),**New Direction in Solid State Chemistry**, Cambridge University Press.
4. Poole, Jr.; Charles P.; Owens, Frank J.:(2003), **Introduction to Nanotechnology**, John Wiley and Sons.
5. Chattopadhyay, K.K.; Banerjee, A. N.(2009),**Introduction to Nanoscience and Technology**, PHI.

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Nanoscale materials and their applications

At least 04 experiments from the following:

1. Synthesis of metal nanoparticles by chemical reduction method.
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. (Students can be provided with XRD patterns of known materials and asked to interpret the data.)
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.

Teaching Learning Process:

Lectures, ICT enabled presentations and group discussions will be part of teaching learning process.

Assessment Methods:

Internal assessment will be through assignments, projects, presentation and class test. End semester examination will be for theory and practical.

Keywords:

Nanomaterials, Preparation, Characterization, Applications.

Course Code: CHEMISTRY –DSE-15

Course Title: Dissertation

Total Credits: 06

Objectives:

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

Learning Outcomes:

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

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

Content:

Unit 1: Identification of research problem

Unit 2: Survey of literature

Unit 3: Formulation of hypothesis, experimental design and methodology

Unit 4: Analysis of data and interpretation of results

Unit 5: Discussion and conclusion

Unit 6: Writing a project report

Assessment Methods:

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

SKILL-ENHANCEMENT COURSES (SEC)

Course Code: CHEMISTRY –SEC-1

Course Title: IT Skills For Chemists

Total Credits: 04

(Credits: Theory-02, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Mathematics

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

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

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

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

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

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

(Lectures: 10)

Unit 2:

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

(Lectures: 4)

Unit 3:

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

(Lectures: 6)

Unit 4:

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

(Lectures: 6)

Unit 5:

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

(Lectures: 4)

Practical:

(Credits: 2, Laboratory periods: 60)

1. Plotting graphs using a spreadsheet
 - i. Planck's distribution law
 - ii. Radial distribution curves for hydrogenic orbitals,
 - iii. Maxwell-Boltzmann distribution curves as function of temperature and molecular weight

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

References:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –SEC-2

Course Title: Basic Analytical Chemistry

Total Credits: 04

(Credits: Theory-02, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Introduction

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

(Lectures: 6)

Unit 2:

Analysis of soil

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

(Lectures: 8)

Unit 3:

Analysis of water:

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

(Lectures:8)

Unit 4:

Chromatography

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

(Lectures: 8)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab-Basic analytical chemistry

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

References:

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

Teaching Learning Process:

- Conventional chalk and board teaching,

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –SEC-3

Course Title: Chemical Technology and Society

Total Credits: 04

(Credits: Theory-04)

(Total Lectures: Theory- 60)

Objectives:

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

Learning Outcomes:

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

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

Chemical Technology

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

Society

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

Sources of energy

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

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

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

Natural Polymers

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

Basics of drug synthesis

Application of genetic engineering

References:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

Chemical Technology; Society; Energy; Polymer; Pollutants.

Course Code: CHEMISTRY –SEC-4

Course Title: Chemoinformatics

Total Credits: 04

(Credits: Theory-02, Practicals-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

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

(Lectures: 2)

Unit 2:

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

(Lectures: 2)

Unit 3:

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

(Lectures: 6)

Unit 4:

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

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(Lectures: 6)

Unit 5:

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

(Lectures: 6)

Unit 6:

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

(Lectures: 8)

Practical:

(Credits: 2, Laboratory periods: 60)

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

- i. Building ab initio
- ii. Building from similar ligands
- iii. Building with a known macromolecular target
- iv. Building without a known macromolecular target
- v. Computational assessment of activity and toxicity and drugability.

References:

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

Additional Resources:

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

Teaching Learning Process:

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

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –SEC-5

Course Title: Business Skills for Chemists

Total Credits: 04

(Credits: Theory-04)

(Total Lecture: Theory-60)

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Chemistry in industry

Current challenges and opportunities for the chemistry based industries.

Role of chemistry in India and global economies.

Chemistry based products in the market.

(Lectures: 10)

Unit 2:

Business Basics

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

(Lectures: 12)

Unit 3:

Project Management

Different stages of a project:

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

(Lectures: 10)

Unit 4:

Commercial Realisation and Case Studies

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

(Lectures: 10)

Unit 5:

Intellectual Property Rights

Introduction to IPR & Patents

(Lectures: 6)

Unit 6:

Environmental Hazards

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

(Lectures: 12)

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

References:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –SEC-6
Course Title: Intellectual Property Rights

Total Credits: 04

(Total Lectures: Theory-60)

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Introduction

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

(Lectures: 8)

Unit 2:

Copyright and Related rights

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

(Lectures: 10)

Unit 3:

Patents

Introduction, Criteria for obtaining patents, Patentable subject matter, Non patentable inventions, Procedure for registration, Term of patent and Rights of patentee, Patent Cooperation Treaty & International registration, Basic concept of Compulsory license and Government use of patent,

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Infringement of patents and remedies, Software patents and importance for India, Utility model & patent, Trade secrets and know-how agreement, Traditional Knowledge and efforts of Indian Govt. for its protection.

(Lectures: 15)

Unit 4:

Trade Marks

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

(Lectures: 8)

Unit 5:

Designs, GI and Plant Varieties Protection

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

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

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

(Lectures: 12)

Unit 6:

Enforcement and Protection

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

(Lectures: 7)

Practical:

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

References:

1. Pandey, N.; Dhama, K. (2014), **Intellectual Property Rights**, PHI Learning Pvt. Ltd.
2. Acharya, N.K.(2001), **Text Book of Intellectual Property Rights**, Asia Law House.

3. Ganguli, P. (2001), **Intellectual Property Rights: unleashing the knowledge economy**. Tata McGraw Hill.

Additional Resources:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –SEC-7

Course Title: Analytical Clinical Biochemistry

Total Credits: 04

(Credits: Theory-02, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

- Demonstrate an understanding of the biochemistry of diseases.
- Understand the application of chemistry in biological systems.

Unit 1:

Metabolism

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

(Lectures: 4)

Unit 2:

Enzymes

Nomenclature, classification, Characterisation, Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, Specificity of enzyme action (Including stereospecificity), Enzyme inhibitors and their importance, Introduction to biocatalysis: Importance in —green chemistry and chemical industry. Drug action-receptor theory. Structure – activity relationships of drug molecules, binding role of –OH group, -NH₂ group, double bond and aromatic ring.

(Lectures: 8)

Unit 3:

Lipids

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

(Lectures: 6)

Unit 4:

Nucleic Acids

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

(Lectures: 6)

Unit 5:

Biochemistry of disease

A diagnostic approach by blood/ urine analysis, Blood: composition and functions of blood, blood coagulation. Blood collection and preservation of samples, Anaemia, Urine: Collection and preservation of samples. Formation of urine. Composition and estimation of constituents of normal and pathological

urine. Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

(Lectures: 6)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Analytical clinical biochemistry

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

References:

Theory:

1. Devlin, T.M. (2010), **Textbook of Biochemistry with Clinical Correlation**, Wiley.
2. Berg, J. M.; Tymoczko, J. L.; Stryer, L. (2002), **Biochemistry**, W. H. Freeman.
3. Satyanarayana, U.; Chakrapani, U. (2017), **Fundamentals of Biochemistry**, Books and Allied (P) Ltd.
4. Lehninger, A.L; Nelson, D.L; Cox, M.M. (2009), **Principles of Biochemistry**, W. H. Freeman.
5. Finar, I. L. **Organic Chemistry** (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Practical:

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

Teaching Learning Process:

- The teaching learning process will involve the traditional chalk and black board method.
- Certain topics like Mechanism of enzyme action, drug receptor theory, transcription and translation, SAR etc. where traditional chalk and talk method may not be able to convey the concept, are taught through audio-visual aids.

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –SEC-8

Course Title: Green Methods in Chemistry

Total Credits: 04

(Credits: Theory-02, Practicals-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Introduction

- Definition of green chemistry and how it is different from conventional chemistry and environmental chemistry.
- Need of green chemistry
- Importance of green chemistry in- daily life, Industries and solving human health problems (four examples each).
- A brief study of Green Chemistry Challenge Awards (Introduction, award categories and study about five last recent awards).**(Lectures:8)**

Unit 2:

Twelve Principles of Green Chemistry

The twelve principles of the Green Chemistry with their explanations

Special emphasis on the following:

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

(Lectures:14)

Unit 3:

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

Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.

Designing of environmentally safe marine antifoulant.

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

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

(Lectures:8)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab- Green methods in chemistry

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

1. Preparation and characterization of nanoparticles of gold using tea leaves/ silver nanoparticles using plant extracts.
2. Preparation and characterization of biodiesel from vegetable oil preferably waste cooking oil.
3. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.
4. 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).
5. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II).
6. Designing and conducting an experiment by utilizing the products and by-products obtained in above preparations which become waste otherwise if not used. This is done by critical thinking and literature survey.

Some representative examples:

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

References:

Theory:

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

Practical:

1. Kirchoff, M.; Ryan, M.A. (2002), **Greener approaches to undergraduate chemistry experiment**. American Chemical Society, Washington DC.
2. Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K.(2013), **Green Chemistry Experiments: A monograph**, I.K. International Publishing House Pvt Ltd. New Delhi.
3. Pavia,D.L.; Lamponam, G.H.; Kriz, G.S.W. B.(2006),**Introduction to organic Laboratory Technique- A Microscale approach**,4th Edition, Brooks-Cole Laboratory Series for Organic chemistry.
4. Sharma R. K., Sharma, C., & Sidhwani, I.T. Solventless and one-pot synthesis of Cu(II) phthalocyanine complex: a green chemistry experiment. Journal of Chemical Education, 2010, 88(1), 86-88.
5. Sharma, R. K., Gulati, S., & Mehta, S. Preparation of gold nanoparticles using tea: a green chemistry experiment. Journal of Chemical Education, 2012, 89(10), 1316-1318.
6. Wealth from waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated "A social Awareness Project" Indu Tucker Sidhwani, Geeta Saini, Sushmita Chowdhury, Dimple Garg, Malovika, Nidhi Garg, Delhi University Journal of Undergraduate Research and Innovation, Vol 1, Issue 1, Feb 2015. ISSN: 2395-2334.

Teaching Learning Process:

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

Assessment Methods:

- Graded assignments
- Conventional class tests

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

Keywords:

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

Course Code: CHEMISTRY –SEC-9

Course Title: Pharmaceutical Chemistry

Total Credits: 04

(Credits: Theory-02, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

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

Unit 1:

Introduction

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

(Lectures: 7)

Unit 2:

Drugs and Pharmaceuticals

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

Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol,

Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), central nervous system agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

(Lectures:15)

Unit 3:

Fermentation

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

(Lectures: 8)

Practical:

(Credits: 2, Laboratory periods: 60)

Chemistry Lab: Pharmaceutical chemistry

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

References:

Theory:

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

Practical:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –SEC-10

Course Title: Chemistry of Cosmetics and Perfumes

Total Credits: 04

(Credits: Theory-02, Practical-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 students of Chemistry honours 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:

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

- Learn basic of cosmetics, various cosmetic formulation, ingredients and their roles in cosmetic products.
- Learn the use of safe, economic and body-friendly cosmetics
- Prepare new innovative formulations.

Unit 1:

Cosmetics- Definition, History, Classification, Ingredients, Nomenclature, Regulations.

(Lectures: 4)

Unit 2:

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

(Lectures: 6)

Unit 3:

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

(Lectures: 5)

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

(Lectures: 6)

Unit 5:

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

(Lectures: 4)

Unit 6:

Personal hygiene products: Antiperspirants and deodorants, oral hygiene products, flavours and essential oils

(Lectures: 5)

Practical:

(Credits: 02, Laboratory periods: 60)

Preparation of:

1. Talcum powder.
2. Shampoo.
3. Enamels.
4. Face cream.
5. Nail polish and nail polish remover.
6. Hand wash
7. Hand sanitizer
8. Body lotion
9. Soap
10. Tooth powder
11. Tooth paste

References:

1. Barel, A.O.; Paye, M.; Maibach, H.I.(2014), **Handbook of Cosmetic Science and Technology**, CRC Press.
2. Garud, A.; Sharma, P.K.; Garud, N. (2012),**Text Book of Cosmetics**, Pragati Prakashan.
3. Gupta, P.K.; Gupta, S.K.(2011),**Pharmaceutics and Cosmetics**, Pragati Prakashan
4. Butler, H. (2000),**Poucher's Perfumes, Cosmetic and Soap**, Springer
5. Kumari, R.(2018),**Chemistry of Cosmetics**, Prestige Publisher.

Additional Resources:

1. Flick,E.W.(1990), **Cosmetic and toiletry formulations**, Noyes Publications / William Andrew Publishing.
2. Natural Ingredients for Cosmetics; EU Survey 2005
3. Formulation Guide for cosmetics; The Nisshin OilliO Group, Ltd.
4. 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:

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

Keywords:

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

Course Code: CHEMISTRY –SEC-11

Course Title: Pesticide Chemistry

Total Credits: 04

(Credits: Theory-02, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

Unit 1:

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

(Lectures:12)

Unit 2:

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

(Lectures:8)

Unit 3:

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

(Lectures:6)

Unit 4:

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

(Lectures:4)

Practical:

(Credits: 2, Laboratory periods: 60)

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

References:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

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

Course Code: CHEMISTRY –SEC-12

Course Title: Fuel Chemistry

Total Credits: 04

(Credits: Theory-02, Practical-02)

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

Objectives:

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

Learning Outcomes:

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

Unit 1:

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

(Lectures:4)

Unit 2:

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

(Lectures:7)

Unit 3:

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

(Lectures:4)

Unit 4:

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

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

(Lectures:6)

Unit 5:

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

(Lectures:4)

Unit 6:

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

Properties of lubricants (viscosity index, cloud point, pour point and aniline Point) and their determination.

(Lectures:5)

Practical:

(Credits: 2, Laboratory periods: 60)

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

Reference:

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

Teaching Learning Process:

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

Assessment Methods:

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

Keywords:

Energy; Fuels; Petroleum; Biofuels; Synthetic Lubricants
