

Choice Based Credit System (CBCS)

UNIVERSITY OF DELHI

FACULTY OF SCIENCE

**UNDERGRADUATE PROGRAMME
(Courses effective from Academic Year 2015-16)**



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

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Undergraduate Programme Secretariat

Preamble

The University Grants Commission (UGC) has initiated several measures to bring equity, efficiency and excellence in the Higher Education System of country. The important measures taken to enhance academic standards and quality in higher education include innovation and improvements in curriculum, teaching-learning process, examination and evaluation systems, besides governance and other matters.

The UGC has formulated various regulations and guidelines from time to time to improve the higher education system and maintain minimum standards and quality across the Higher Educational Institutions (HEIs) in India. The academic reforms recommended by the UGC in the recent past have led to overall improvement in the higher education system. However, due to lot of diversity in the system of higher education, there are multiple approaches followed by universities towards examination, evaluation and grading system. While the HEIs must have the flexibility and freedom in designing the examination and evaluation methods that best fits the curriculum, syllabi and teaching-learning methods, there is a need to devise a sensible system for awarding the grades based on the performance of students. Presently the performance of the students is reported using the conventional system of marks secured in the examinations or grades or both. The conversion from marks to letter grades and the letter grades used vary widely across the HEIs in the country. This creates difficulty for the academia and the employers to understand and infer the performance of the students graduating from different universities and colleges based on grades.

The grading system is considered to be better than the conventional marks system and hence it has been followed in the top institutions in India and abroad. So it is desirable to introduce uniform grading system. This will facilitate student mobility across institutions within and across countries and also enable potential employers to assess the performance of students. To bring in the desired uniformity, in grading system and method for computing the cumulative grade point average (CGPA) based on the performance of students in the examinations, the UGC has formulated these guidelines.

CHOICE BASED CREDIT SYSTEM (CBCS):

The CBCS provides an opportunity for the students to choose courses from the prescribed courses comprising core, elective/minor or skill based courses. The courses can be evaluated following the grading system, which is considered to be better than the conventional marks system. Therefore, it is necessary to introduce uniform grading system in the entire higher education in India. This will benefit the students to move across institutions within India to begin with and across countries. The uniform grading system will also enable potential employers in assessing the performance of the candidates. In order to bring uniformity in evaluation system and computation of the Cumulative Grade Point Average (CGPA) based on student's performance in examinations, the UGC has formulated the guidelines to be followed.

Outline of Choice Based Credit System:

- 1. Core Course:** A course, which should compulsorily be studied by a candidate as a core requirement is termed as a Core course.
- 2. Elective Course:** Generally a course which can be chosen from a pool of courses and which may be very specific or specialized or advanced or supportive to the discipline/ subject of study or which provides an extended scope or which enables an exposure to some other discipline/subject/domain or nurtures the candidate's proficiency/skill is called an Elective Course.
 - 2.1 Discipline Specific Elective (DSE) Course:** Elective courses may be offered by the main discipline/subject of study is referred to as Discipline Specific Elective. The University/Institute may also offer discipline related Elective courses of interdisciplinary nature (to be offered by main discipline/subject of study).
 - 2.2 Dissertation/Project:** An elective course designed to acquire special/advanced knowledge, such as supplement study/support study to a project work, and a candidate studies such a course on his own with an advisory support by a teacher/faculty member is called dissertation/project.
 - 2.3 Generic Elective (GE) Course:** An elective course chosen generally from an unrelated discipline/subject, with an intention to seek exposure is called a Generic Elective.

P.S.: A core course offered in a discipline/subject may be treated as an elective by other discipline/subject and vice versa and such electives may also be referred to as Generic Elective.
- 3. Ability Enhancement Courses (AEC)/Competency Improvement Courses/Skill Development Courses/Foundation Course:** The Ability Enhancement (AE) Courses may be of two kinds: AE Compulsory Course (AECC) and AE Elective Course (AEEC). "AECC" courses are the courses based upon the content that leads to Knowledge enhancement. They ((i) Environmental Science, (ii) English/MIL Communication) are mandatory for all disciplines. AEEC courses are value-based and/or skill-based and are aimed at providing hands-on-training, competencies, skills, etc.
 - 3.1 AE Compulsory Course (AECC):** Environmental Science, English Communication/MIL Communication.
 - 3.2 AE Elective Course (AEEC):** These courses may be chosen from a pool of courses designed to provide value-based and/or skill-based instruction.

Project work/Dissertation is considered as a special course involving application of knowledge in solving / analyzing /exploring a real life situation / difficult problem. A Project/Dissertation work would be of 6 credits. A Project/Dissertation work may be given in lieu of a discipline specific elective paper.

Details of Courses Under Undergraduate Programme (B.Sc.)

Course	*Credits	
=====		
	Theory+ Practical	Theory+Tutorials
<u>I. Core Course</u>	12X4= 48	12X5=60
(12 Papers)		
04 Courses from each of the		
03 disciplines of choice		
Core Course Practical / Tutorial*	12X2=24	12X1=12
(12 Practical/ Tutorials*)		
04 Courses from each of the		
03 Disciplines of choice		
 <u>II. Elective Course</u>	 6x4=24	 6X5=30
(6 Papers)		
Two papers from each discipline of choice		
including paper of interdisciplinary nature.		
Elective Course Practical / Tutorials*	6 X 2=12	6X1=6
(6 Practical / Tutorials*)		
Two Papers from each discipline of choice		
including paper of interdisciplinary nature		
<ul style="list-style-type: none"> • Optional Dissertation or project work in place of one Discipline elective paper (6 credits) in 6th Semester 		
 <u>III. Ability Enhancement Courses</u>		
1. Ability Enhancement Compulsory	2 X 2=4	2X2=4
(2 Papers of 2 credits each)		
Environmental Science		
English/MIL Communication		
2. Ability Enhancement Elective	4 X 2=8	4 X 2=8
(Skill Based)		
(4 Papers of 2 credits each)		
	_____	_____
	Total credit= 120	Total credit= 120

Institute should evolve a system/policy about ECA/ General Interest/Hobby/Sports/NCC/NSS/related courses on its own.

*wherever there is practical there will be no tutorials and vice -versa

DETAILS OF COURSES

CORE COURSES: Analytical Chemistry

1. Analytical Chemistry: Basic Principles and Laboratory Operations.
2. Separation Methods -1 (General chromatography, Centrifugation, Dialysis)
3. Quantitative Methods of Analysis
4. Separation Methods-2

CORE COURSES: Chemistry

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

CORE COURSES: Matho-Physics

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

DISCIPLINE SPECIFIC ELECTIVES: Analytical Chemistry (Any two)

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

DISCIPLINE SPECIFIC ELECTIVES Chemistry (Any two)

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

DISCIPLINE SPECIFIC ELECTIVES Matho-Physics

(One each from Maths and Physics)

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

ABILITY ENHANCEMENT COMPULSORY COURSES

1. Environmental Science
2. English/ MIL communication

SKILL ENHANCEMENT COURSES (Any four)

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

Scheme of B.Sc Programme (Applied Physical Sciences) Analytical Chemistry

Semester	Course Opted	Course name	Credits	
I	Ability Enhancement	English Communication	2	
	Compulsory Course-1	Environmental Science	2	
	Core Course Analytical Chemistry I	Basic Principles & Laboratory Operations	4	
	Core Course Analytical Chemistry I Practical	Basic Principles & Laboratory Operations Practical	2	
	Core Course Chemistry I	Atomic structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons	4	
	Core Course Chemistry I Practical	Atomic structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons Practical	2	
	Core Course Physics I	Mechanics	4	
	Core Course Physics I Practical	Mechanics Practical	2	
	II	Ability Enhancement	English Communication	2
		Compulsory Course-1	Environmental Science	2
Core Course Analytical Chemistry 2		Separation Methods -1	4	
Core Course Analytical Chemistry 2 Practical		Separation Methods -1 Practical	2	
Core Course Chemistry 2		Chemical Energetics, Equilibria & Functional Group Organic Solutions, Phase Equilibria	4	
Core Course Chemistry 2 Practical		Chemical Energetics, Equilibria & Functional Group Organic Solutions, Phase Equilibria -Practical	2	
Core Course Mathematics 1		Calculus and matrices	4	
III		Core Course Analytical Chemistry3	Quantitative Methods of Analysis	4
	Core Course Analytical Chemistry 3 Practical	Quantitative Methods of Analysis Practical	2	

Semester	Course Opted	Course Name	Credits
	Core Course Chemistry 3 Practical	Conductance, Electrochemistry & Functional Group Organic Chemistry Practical	2
	Core Course Mathematics 2	Algebra	4
	Skill Enhancement Course 1		
IV	Core Course Analytical Chemistry 4	Separation Methods -2	4
	Core Course Analytical Chemistry 4 Practical	Separation Methods -2 Practical	2
	Core Course Chemistry 4	Chemistry of s- and p-block elements, States of matter & Chemical kinetics	4
	Core Course Chemistry 4 Practical	Chemistry of s- and p-block elements, States of matter & Chemical kinetics -Practical	2
	Core Course Physics 2	Wave and optics	4
	Core Course Physics 2 Practical	Wave and optics practical	2
	Skill Enhancement Course -2		2
V	DSE Analytical Chemistry 1		4
	DSE Analytical Chemistry Practical 1		2
	DSE Chemistry 1		4
	DSE Chemistry 1 Practical		2
	DSE Physics 1		4
	DSE Physics 1 Practical		2
	Skill Enhancement Course 3		2
VI	DSE Analytical Chemistry 2		4
	DSE Analytical Chemistry 2 Practical		2
	DSE Chemistry 2		4
	DSE Chemistry 2 Practical		2
	DSE Mathematics 1		4
	Skill Enhancement Course 4		2

SEMESTER –I

(CORE COURSE ANALYTICAL CHEMISTRY -1) (Credits: Theory-04, Practicals-02)

ANALYTICAL CHEMISTRY-1: BASIC PRINCIPLES & LABORATORY OPERATIONS

I. Basic Concepts:

A. Système international d'unités or SI Units

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

B. Chemical concentrations

- i. Mole, molar mass
- ii. Calculations in grams and moles
- iii. Solutions and their concentrations:
 - a) Molar concentration b) Analytical molarity c) Equilibrium molarity of a particular species d) Percent concentration e) Parts per million/billion (ppm, ppb) f) Volume ratios for dilution procedures g) p-functions.

C. Preparing solutions: standard solutions, primary standards, secondary standards.

II. Introduction to Analytical Chemistry and Analytical Methods

- i. General steps in chemical analysis
- ii. Introduction to methods of detecting analytes a) Physical b) Electromagnetic radiations c) Electric charge

III. Laboratory Operations

- i. Description and use of common laboratory apparatus: Volumetric flasks, burettes, Pipettes, meniscus readers, weighing bottles, different types of funnels chromatographic columns, chromatographic jars, desiccators, drying ovens, filter crucibles, rubber policeman.
- ii. Calibration and use of volumetric glass ware.
- iii. pH meter: components of pH meter use of pH Meter, maintenance of pH meter, application of data.
- iv. Laboratory notebook.

IV. Errors in Chemical Analysis

- i. Types of errors
- ii. Accuracy and Precision, Absolute and relative uncertainty, propagation of uncertainty.
- iii. The Gaussian distribution, mean and standard deviation, confidence intervals.
- iv. Statistical tests of data (the F test, the t test, Q test for bad data, the method of least squares).
- v. Calibration curve.
- vi. Safety with chemicals and waste.

Analytical Chemistry Lab -1: Basic Principles & Laboratory Operations

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

Suggested Readings:

1. Seamus P.J. Higson: Analytical Chemistry.
2. Douglas A. Skoog and Donald M. West: Fundamentals of Analytical Chemistry.
3. Adion A. Gordus: Schaum's Outline of Analytical Chemistry, Tata McGraw-Hill.
4. Gary D. Christian: Analytical Chemistry.
5. Freifelder and Kealy: Analytical Chemistry.
6. Daniel C Harris: Exploring Chemical Analysis.
7. Daniel C Harris: Quantitative Chemical Analysis

(CORE COURSE CHEMISTRY I)

CHEMISTRY: ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS (Credits: Theory-04, Practicals-02)

Section A: Inorganic Chemistry-1 (30 Periods)

Atomic Structure: Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de-Broglie's relation, Heisenberg Uncertainty principle. 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.

(14 Lectures)

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, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Covalent bonding: VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR 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⁺. Comparison of VB and MO approaches.

(16 Lectures)

Section B: Organic Chemistry-1 (30 Periods)

Fundamentals of Organic Chemistry

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis. Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals. Strength of organic acids and bases: Comparative

study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule.

(8 Lectures)

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).

(10 Lectures)

Aliphatic Hydrocarbons

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Alkanes: (Upto 5 Carbons). *Preparation:* Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. *Reactions:* Free radical Substitution; Halogenations.

Alkenes: (Upto 5 Carbons) *Preparation:* Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); *cis* alkenes (Partial catalytic hydrogenation) and *trans* alkenes (Birch reduction). *Reactions:* *cis*-addition (alk. KMnO₄) and *trans*-addition (bromine), Addition of HX (Markownikoff's and anti- Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation.

Alkynes: (Upto 5 Carbons) *Preparation:* Acetylene from CaC₂ and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal dihalides.

Reactions: formation of metal acetylides, addition of bromine and alkaline KMnO₄, ozonolysis and oxidation with hot alk. KMnO₄.

(12 Lectures)

Reference Books:

1. J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
2. F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
3. Douglas, McDaniel and Alexander: *Concepts and Models in Inorganic Chemistry*, John Wiley.
4. James E. Huheey, Ellen Keiter and Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
5. T. W. Graham Solomon: *Organic Chemistry*, John Wiley and Sons.
6. Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
7. E. L. Eliel: *Stereochemistry of Carbon Compounds*, Tata McGraw Hill.
8. I. L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
9. R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
10. Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand

Chemistry Lab – 1 Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons

60 Lectures

Section A: Inorganic Chemistry - Volumetric Analysis

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with KMnO₄.
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO₄.
4. Estimation of Fe (II) ions by titrating it with K₂Cr₂O₇ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using Na₂S₂O₃.

Section B: Organic Chemistry

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)
2. 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 paper chromatography
 - (b) Identify and separate the sugars present in the given mixture by paper chromatography.

Reference Books:

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

(CORE COURSE PHYSICS -1)
MECHANICS
(Credits: Theory-04, Practicals-02)

Vectors: Vector algebra. Scalar and vector products. Derivatives of a vector with respect to a parameter. (4 Lectures)

Ordinary Differential Equations:

1st order homogeneous differential equations. 2nd order homogeneous differential equations with constant coefficients. (6 Lectures)

Laws of Motion:

Frames of reference. Newton's Laws of motion. Dynamics of a system of particles. Centre of Mass. (10 Lectures)

Momentum and Energy:

Conservation of momentum. Work and energy. Conservation of energy. Motion of rockets. (6 Lectures)

Rotational Motion:

Angular velocity and angular momentum. Torque. Conservation of angular momentum. (5 Lectures)

Gravitation:

Newton's Law of Gravitation. Motion of a particle in a central force field (motion is in a plane, angular momentum is conserved, areal velocity is constant). Kepler's Laws (statement only). Satellite in circular orbit and applications. Geosynchronous orbits. Weightlessness. Basic idea of global positioning system (GPS). Physiological effects on astronauts. (8 Lectures)

Oscillations:

Simple harmonic motion. Differential equation of SHM and its solutions. Kinetic and Potential Energy, Total Energy and their time averages. Damped oscillations. (6 Lectures)

Elasticity: Hooke's law - Stress-strain diagram - Elastic moduli-Relation between elastic constants - Poisson's Ratio-Expression for Poisson's ratio in terms of elastic constants - Work done in stretching and work done in twisting a wire - Twisting couple on a cylinder Determination of Rigidity modulus by static torsion - Torsional pendulum-Determination of Rigidity modulus and moment of inertia - q , η and σ by Searles method (8 Lectures)

Speed Theory of Relativity:

Constancy of speed of light. Postulates of Special Theory of Relativity. Length contraction. Time dilation. Relativistic addition of velocities. (7 Lectures)

Note: Students are not familiar with vector calculus. Hence all examples involve differentiation either in one dimension or with respect to the radial coordinate.

Reference Books:

1. University Physics. FW Sears, MW Zemansky and HD Young 13/e, 1986. Addison-Wesley
2. Mechanics Berkeley Physics course, v.1: Charles Kittel, et. Al. 2007, Tata McGraw-Hill.
3. Physics – Resnick, Halliday & Walker 9/e, 2010, Wiley
4. University Physics, Ronald Lane Reese, 2003, Thomson Brooks/Cole.

Physics Lab- 1: Mechanics

60 Lectures

1. Measurements of length (or diameter) using vernier caliper, screw gauge and travelling microscope.
2. To determine the Height of a Building using a Sextant.
3. To determine the Moment of Inertia of a Flywheel.
4. To determine the Young's Modulus of a Wire by Optical Lever Method.
5. To determine the Modulus of Rigidity of a Wire by Maxwell's needle.
6. To determine the Elastic Constants of a Wire by Searle's method.
7. To determine g by Bar Pendulum.
8. To determine g by Kater's Pendulum.
9. To determine g and velocity for a freely falling body using Digital Timing Technique
10. To study the Motion of a Spring and calculate (a) Spring Constant (b) Value of g

Reference Books:

1. Advanced Practical Physics for students, B.L.Flint and H.T.Worsnop, 1971, Asia Publishing House.
2. Advanced level Physics Practicals, Michael Nelson and Jon M. Osborn, 4th Edition, reprinted 1985, Heinemann Educational Publishers
3. A Text Book of Practical Physics, Indu Prakash and Ramakrishna, 11th Edition, 2011, Kitab Mahal, New Delhi.

SEMESTER II

CORE COURSE ANALYTICAL CHEMISTRY -2

SEPARATION METHODS – I (Theory 04 credits, Practicals 02 credits)

I. Chromatography:

- A. Classification of chromatographic methods: Principle of differential migration, description of the chromatographic process, distribution coefficients, modes of chromatography, performing column chromatography.
- B. Chromatography – theory and practice: Introduction, the chromatograph (elution time and volume), capacity factor, column efficiency and resolution, sample preparation
- C. Techniques of paper chromatography: experimental modifications, various modes of development, nature of the paper, detection of spots, retardation factors, factors that affect the reproducibility of R_f values (due to paper, solvent system, sample, development procedure), selection of solvent, quantitative analysis. applications
- D. Thin layer chromatography: stationary phase, adsorbents, liquid phase supports, plate preparation, mobile phase, sample application, development, saturation of chamber, detection of spot, R_f values (effect of adsorbent, solvent, solute, development process), quantitative analysis, applications

II. Solvent Extraction:

Distribution law, Determination of distribution ratio, Batch extraction, continuous extraction, discontinuous extraction, counter current extraction

III. Dialysis and Membrane Filtration

General laboratory methods, Filters – nitrocellulose, fibreglass, polycarbonates.

Analytical Chemistry Lab - 2: Separation Methods-1

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

Suggested Readings:

- 1. F.W. Fifield and D. Kealy : Analytical Chemistry.
- 2. Daniel C Harris: Exploring chemical analysis.
- 3. Daniel C Harris: Quantitative chemical analysis.
- 4. R.V. Dilts Analytical Chemistry- Methods of Separation.
- 5. O. Mikes, R.A. Chalmers: Laboratory Handbook of Chromatographic Methods.

CORE COURSE CHEMISTRY-2

CHEMISTRY: CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY

(Credits: Theory-04, Practicals-02)

Section A: Physical Chemistry-1 (30 Lectures)

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. (10 Lectures)

Chemical Equilibrium:

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔG° , Le Chatelier's principle. Relationships between K_p , K_c and K_x for reactions involving ideal gases.

(8 Lectures)

Ionic Equilibria:

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. (12 Lectures)

Section B: Organic Chemistry-2

(30 Lectures)

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Aromatic hydrocarbons

Preparation (Case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid.

Reactions: (Case benzene): Electrophilic substitution: nitration, halogenation and sulphonation. Friedel-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (upto 4 carbons on benzene).

(8 Lectures)

Alkyl and Aryl Halides

Alkyl Halides (Upto 5 Carbons) Types of Nucleophilic Substitution (SN_1 , SN_2 and SN_i) reactions.

Preparation: from alkenes and alcohols.

Reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation.

Williamson's ether synthesis: Elimination vs. substitution.

Aryl Halides Preparation: (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions.

Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by $-OH$ group) and effect of nitro substituent. Benzyne Mechanism: KNH_2/NH_3 (or $NaNH_2/NH_3$). Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

(8 Lectures)

Alcohols, Phenols and Ethers (Upto 5 Carbons)

Alcohols: *Preparation*: Preparation of 1o, 2o and 3o alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters.

Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. KMnO_4 , acidic dichromate, conc. HNO_3). Oppeneauer oxidation *Diols*: (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement.

Phenols: (Phenol case) *Preparation*: Cumene hydroperoxide method, from diazonium salts.

Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben-Hoesch Condensation, Schotten – Baumann Reaction.

Ethers (aliphatic and aromatic): Cleavage of ethers with HI.

Aldehydes and ketones (aliphatic and aromatic): (Formaldehyde, acetaldehyde, acetone and benzaldehyde)

Preparation: from acid chlorides and from nitriles.

Reactions – Reaction with HCN, ROH, NaHSO_3 , NH_2 -G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Ponndorf Verley reduction.

(14 Lectures)

Reference Books:

1. T. W. Graham Solomons: *Organic Chemistry*, John Wiley and Sons.
2. Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
3. I.L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.19
4. R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
5. Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand.
6. G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
7. G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).
8. J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
9. B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
10. R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).

Chemistry Lab - 2: Chemical Energetics, Equilibria & Functional Organic Chemistry 60 Lectures

Section A: Physical Chemistry

Thermochemistry

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts (KNO_3 , NH_4Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of ΔH .
Ionic equilibria, pH measurements
 - a) Measurement of pH of different solutions like aerated drinks, fruit juices, shampoos and soaps (use dilute solutions of soaps and shampoos to prevent damage to the glass electrode) using pH-meter.
 - b) Preparation of buffer solutions:
 - (i) Sodium acetate-acetic acid

(ii) Ammonium chloride-ammonium hydroxide

Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

Section B: Organic Chemistry

1. Purification of organic compounds by crystallization (from water and alcohol) and distillation.

2. Criteria of Purity: Determination of melting and boiling points.

3. Preparations: Mechanism of various reactions involved to be discussed.

Recrystallisation, determination of melting point and calculation of quantitative yields to be done.

(a) Bromination of Phenol/Aniline

(b) Benzoylation of amines/phenols

(c) Oxime and 2,4 dinitrophenylhydrazone of aldehyde/ketone

Reference Books

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

CORE COURSE MATHEMATICS -1

MATHEMATICS -Paper I (4 credits) CALCULUS AND MATRICES

Unit I. Matrices R , R^2 , R^3 as vector spaces over R . Standard basis for each of them. Concept of Linear Independence and examples of different bases. Subspaces of R^2 , R^3 . Translation, Dilation, Rotation, Reflection in a point, line and plane. Matrix form of basic geometric transformations. Interpretation of eigenvalues and eigenvectors for such transformations and eigenspaces as invariant subspaces. Matrices in diagonal form. Reduction to diagonal form upto matrices of order 3. Computation of matrix inverses using elementary row operations. Rank of matrix. Solutions of a system of linear equations using matrices. Illustrative examples of above concepts from Geometry, Physics, Chemistry, Combinatorics and Statistics.

Unit II. Calculus Sequences to be introduced through the examples arising in Science beginning with finite sequences, followed by concepts of recursion and difference equations. For instance, the sequence arising from Tower of Hanoi game, the Fibonacci sequence arising from branching habit of trees and breeding habit of rabbits. Convergence of a sequence and algebra of convergent sequences. Illustration of proof of convergence of some simple sequences such as $(-1)^n/n$, $1/n^2$, $(1+1/n)^n$, $\sin n/n$, x^n with $0 < x < 1$. Graphs of simple concrete functions such as polynomial, trigonometric, inverse trigonometric, exponential, logarithmic and hyperbolic functions arising in problems or chemical reaction, simple pendulum, radioactive decay, temperature cooling/heating problem and biological rhythms. Successive differentiation. Leibnitz theorem. Recursion formulae for higher derivative. Functions of two variables. Graphs and Level Curves of functions of two variables. Partial differentiation upto second order. Computation of Taylor's Maclaurin's series of functions such as e^x , $\log(1+x)$, $\sin(2x)$, $\cos x$. Their use in polynomial approximation and error estimation. Formation and solution of Differential equations arising in population growth, radioactive decay, administration of medicine and cell division. 4

Unit III. Geometrical representation of addition, subtraction, multiplication and division of complex numbers. Lines half planes, circles, discs in terms of complex variables. Statement of the Fundamental Theorem of Algebra and its consequences, De Moivre's theorem for rational indices and its simple applications.

Recommended Books :

1. George B. Thomas, Jr., Ross L. Finney : Calculus and Analytic Geometry, Pearson Education (Singapore); 2001.
2. T.M. Apostol : Calculus, vol. 1, John Wiley and Sons (Asia) : 2002.
3. A.I. Kostrikin: Introduction to Algebra, Springer Verlag, 1984

SEMESTER III

CORE COURSE ANALYTICAL CHEMISTRY -3

QUANTITATIVE METHODS OF ANALYSIS

(Theory 04 credits, Practical 02 credits)

I. Gravimetric Analysis:

- A. Precipitation methods
- B. Volatilization methods. (The analyte or its decomposition products are volatilized at a suitable temperature. The volatile product is then collected and weighed, or, alternatively, the mass of the product is determined indirectly from the loss in mass of the sample. e.g., determination of the sodium hydrogen carbonates content of antacid tablets)
- C. Properties of precipitates and precipitating reagents:
 - Particle size, Filterability of Precipitates (factors that determine particle size, formation of precipitates and particle size).
 - Colloidal Precipitates (coagulation of colloids, peptization of colloids, treatment of colloidal precipitates).
 - Crystalline Precipitates (particle size and filterability).
 - Co-precipitation (surface adsorption, mixed-crystal formation, occlusion, and mechanical entrapment, co precipitation errors).
 - Precipitation from Homogeneous Solution (The use of the technique of homogeneous solutions to effect precipitation).
- D. Drying and Ignition of precipitates
- E. Practical gravimetric procedures.

II. Volumetric Analysis

- A. Definitions: Titrimetry, Volumetric titrimetry, Gravimetric titrimetry, Coulometric titrimetry. The equivalence point, the end point
- B. Volumetric methods of analysis: Classification of volumetric methods, theory of indicators and buffers. Equilibria, Principles, Aqueous and non-aqueous acid-base titration. Redox titrations. Complexometric titrations. Precipitation titrations
- C. Typical problems in volumetric titrimetry:
- D. Sigmoidal Titration Curves
- E. The Henderson-Hasselbalch Equation.

III. Centrifugation Methods:

- A. Introduction
- B. Sedimentation and relative centrifugal force
- C. Different types of rotors.
- D. Density gradient
- E. Types of centrifugation techniques.

IV. Introduction to Environmental Analysis:

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

Analytical Chemistry Lab 3 : Quantitative Methods of Analysis

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

Suggested Readings:

1. Analytical Chemistry- Methods of Separation (R. V. Dilts).
2. Laboratory Handbook of Chromatographic Methods (O. Mikes, R.A. Chalmers).
3. F.W. Fifield and D. Kealy: Analytical Chemistry.
4. Vogel's textbook of quantitative chemical analysis, 6th edition.
5. Vogel's textbook of quantitative chemical analysis, 7th edition.
6. Keith Wilson and John Walker: Practical Biochemistry.

CORE COURSE CHEMISTRY-3

SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY & FUNCTIONAL GROUP ORGANIC CHEMISTRY-II (Credits: Theory-4, Practicals-2)

Section A: Physical Chemistry-2 (30 Lectures)

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.

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).

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

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. Thermodynamicsof areversible 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).

Section B: Organic Chemistry-3

(30 Lectures)

Functional group approach for the following reactions (preparations Physical Property & Chemicals reactions) to be studied in context to their structure with mechanism.

Carboxylic acids and their derivatives

Carboxylic acids (aliphatic and aromatic)

Preparation: Acidic and Alkaline hydrolysis of esters.

Reactions: Hell – Vohlard - Zelinsky Reaction, Acidity of carboxylic acid, effect of substitution on acid strength.

Carboxylic acid derivatives (aliphatic):

Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion claisen condensation.

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

Amines and Diazonium Salts

Amines (Aliphatic and Aromatic):

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 basic character of amines. .

Diazonium salts: *Preparation:* from aromatic amines.

Reactions: conversion to benzene, phenol, dyes.

Amino Acids, Peptides and Proteins:

Zwitterion, Isoelectric point and Electrophoresis

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

Reactions of Amino acids: ester of $-\text{COOH}$ 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.

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.

Reference Books:

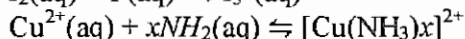
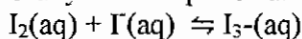
1. M. Barrow: *Physical Chemistry* Tata McGraw Hill (2007).
2. W. Castellán: *Physical Chemistry* 4th Ed. Narosa (2004).
3. C. Kotz, P. M. Treichel, J. R. Townsend, *General Chemistry*, Cengage Learning India Pvt. Ltd.: New Delhi (2009).
4. H. Mahan: *University Chemistry*, 3rd Edn. Narosa (1998).
5. H. Petrucci, *General Chemistry*, 5th Edn., Macmillan Publishing Co.: New York (1985).
6. Morrison R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
7. Finar I. L. *Organic Chemistry* (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
8. Finar I. L. *Organic Chemistry* (Volume 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
9. Nelson D. L. & Cox, M. M. *Lehninger's Principles of Biochemistry* 7th Ed., W. H. Freeman.
10. Berg J. M., Tymoczko, J. L. & Stryer, L. *Biochemistry* 7th Ed., W. H. Freeman

Chemistry Lab 3: Solutions, Phase Equilibrium, Conductance, Electrochemistry & Biomolecules

Section A: Physical Chemistry

Distribution

Study of the equilibrium of one of the following reactions by the distribution method:



Phase equilibria

- Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.
- Determination of the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.
- Study of the variation of mutual solubility temperature with concentration for the phenol water system and determination of the critical solubility temperature.

Conductance

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

Potentiometry

Perform the following potentiometric titrations:

- Strong acid vs. strong base
- Weak acid vs. strong base
- Potassium dichromate vs. Mohr's salt

Section B: Organic Chemistry

I Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (amide, nitro, amines, Hydrocarbons, Halo Hydrocarbons) and preparation of one derivative.

II

- Determination of the concentration of glycine solution by formylation method
- Action of salivary amylase on starch
- Differentiation between a reducing and nonreducing sugar

Reference Books:

- A.I. Vogel: Textbook of Practical Organic Chemistry, Prentice Hall, 5th Edn.
- F.G. Mann & B. C. Saunders: Practical Organic Chemistry, Orient Longman, 1960.
- B.D. Khosla: Senior Practical Physical Chemistry, R. Chand & Co.
- Ahluwalia V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.

CORE COURSE MATHEMATICS -2

ALGEBRA

(Credits-04)

Groups: Definition and examples of groups, examples of abelian and nonabelian groups: the group Z_n of integers under addition modulo n and the group $U(n)$ of units under multiplication modulo n . Cyclic groups from number systems, complex roots of unity, circle group, the general linear group $GL(n, R)$, groups of symmetries of (i) an isosceles triangle, (ii) an equilateral triangle, (iii) a rectangle, and (iv) a square, the permutation group $Sym(n)$, Group of quaternions, Subgroups, cyclic subgroups, the concept of a subgroup generated by a subset and the commutator subgroup of group, examples of subgroups including the center of a group. Cosets, Index of subgroup, Lagrange's theorem, order of an element, Normal subgroups: their definition, examples, and characterizations, Quotient groups.

Rings: Definition and examples of rings, examples of commutative and noncommutative rings, rings from number systems, Z_n the ring of integers modulo n , ring of real quaternions, rings of matrices, polynomial rings, and rings of continuous functions. Subrings and ideals, Integral domains and fields, examples of fields: Z_p , Q , R , and C . Field of rational functions. Vector spaces: Definition and examples of vector spaces. Subspaces and its properties Linear independence, basis, invariance of basis size, dimension of a vector space. Linear Transformations on real and complex vector spaces: definition, examples, kernel, range, rank, nullity, isomorphism theorems.

References:

1. Joseph A Gallian: Contemporary Abstract Algebra, fourth edition, Narosa, 1999.
2. George E Andrews: Number Theory, Hindustan Publishing Corporation, 1984
3. C.W. Curtis, Linear Algebra, an introductory approach, SpringerVerlag, 1991.
4. David M. Blotin, Linear algebra and Geometry, Cambridge Press, 1979.

SEMESTER IV

CORE COURSE ANALYTICAL CHEMISTRY- 4 (Theory 04 credits, Practicals 02 Credits)

SEPARATION METHODS - II

I. Column Chromatography.

- A. General: columns, matrix materials, stationary phase, column packing, application of sample, column development and sample elution, detectors and fraction collectors, applications.
- B. High performance liquid chromatography: Principle, column, matrices and stationary phases, column packing, mobile phase and pumps, application of sample, detectors, applications.
- C. Adsorption chromatography: Principle, adsorbents, solvents, nature of solute, operating parameters, retention volumes and times, applications.
- D. Liquid-liquid partition, chromatography: Principle, normal phase chromatography, reversed- phase liquid chromatography, reversed phase liquid chromatography, applications.
- E. Ion- exchange chromatography: Principle, ion exchangers, ion- exchange equilibria, ion-exchange resin selectivity, column operations (column development, detection of solute bands), factors affecting retention volumes, applications.
- F. Gel chromatography: Principle, types of gels, separation by gel chromatography, applications.
- G. Affinity chromatography: Principle, materials, selection and attachment of ligand, practical procedure, applications,
- H. Gas- liquid chromatography: Apparatus and materials, preparation and application of samples, separation conditions, detectors, applications.

II. Electrophoretic Techniques:

- A. Principle, apparatus, support media (paper, cellulose acetate membranes, gels).
- B. SDS-PAGE, native gels, gradient gels, isoelectric focusing, 2D-PAGE, continuous flow electrophoresis, detection, estimation and recovery of proteins in gels.
- C. Western blotting, electrophoresis of nucleic acids, capillary electrophoresis.
- D. Isoelectric Focusing

III. Radioisotopic Techniques: nature of radioactivity. Detection and measurement of radioactivity, inherent advantages and restrictions of radiotracer experiments, safety aspects.

Analytical Chemistry Lab 4: Separation Methods-2

1. Determination of residual chlorine in city water supply using colorimetry.
2. Determination of adsorption isotherm of acetic acid on activated charcoal and determination of the adsorption constant (k).
3. Determination of the capacity of an anion exchange resin.
4. Determination of the capacity of a cation exchange resin.
5. Separation of compounds using adsorption column chromatography.
6. Determination of isoelectric point of an amino acid.
7. Determination of void volume of a gel column.

Suggested Readings:

1. R.V.Dilts: Analytical Chemistry- Methods of Separation.
2. O. Mikes, R.A. Chalmers: Laboratory Handbook of Chromatographic Methods.
3. F.W. Fifield and D.Kealy: Principles and practice of analytical chemistry.
4. Vogel's textbook of quantitative chemical analysis, 6th edition.
5. Vogel's textbook of quantitative chemical analysis, 7th edition.
6. Keith Wilson and John Walker: Practical Biochemistry.
7. David J.Holme and Hazel Peck: Analytical Biochemistry.
8. David Freifelder: Physical Biochemistry.
9. Practical Biochemistry : D.T. Plummer
10. Practical Biochemistry: Jayram

CORE COURSE CHEMISTRY -4

CHEMISTRY OF S- AND P-BLOCK ELEMENTS, STATES OF MATTER & CHEMICAL KINETICS (Credits: Theory-4, Practicals-2)

Section A: Inorganic Chemistry

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 and Mond's process. (4 Lectures)

s- and *p*-Block Elements

Periodicity in *s*- and *p*-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electro negativity (Pauling, Mulliken, and Alfred-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 (NH₃, N₂H₄, N₃H, NH₂OH) Oxoacids of P, S and Cl. Halides and oxohalides: PCl₃, PCl₅, SOCl₂ and SO₂Cl₂ (26 Lectures)

Section B: Physical Chemistry-3 (30 Lectures)

Kinetic Theory of Gases

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation. Deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. van der Waals equation of state for real gases. Boyle temperature (derivation not required). Critical phenomena, critical constants and their calculation from van der Waals equation. Andrews isotherms of CO₂.

Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance.

Temperature dependence of these distributions. Most probable, average and root mean square velocities (no derivation). Collision cross section, collision number, collision frequency, collision diameter and mean free path of molecules. Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only).

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)

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.

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 bimolecular reactions. Comparison of the two theories (qualitative treatment only).

Reference Books:

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

Chemistry Lab 4: Chemistry of s- AND p-Block Elements, States of Matter & Chemical Kinetics

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⁺, Ag⁺, Bi³⁺, Cu²⁺, Cd²⁺, Sn²⁺, Fe³⁺, Al³⁺, Co²⁺, Cr³⁺, Ni²⁺, Mn²⁺, Zn²⁺, Ba²⁺, Sr²⁺, Ca²⁺, K⁺

Anions : CO₃²⁻, S²⁻, SO₂⁻, S₂O₃²⁻, NO₃⁻, CH₃COO⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, SO₄²⁻, PO₄³⁻, BO₃³⁻, C₂O₄²⁻, F⁻

(Spot tests should be carried out wherever feasible)

Section B: Physical Chemistry

(I) Surface tension measurement (use of organic solvents excluded).

- a) Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.
- b) Study of the variation of surface tension of a detergent solution with concentration.

(II) Viscosity measurement (use of organic solvents excluded).

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

(III) Chemical Kinetics

Study the kinetics of the following reactions.

1. Initial rate method: Iodide-persulphate reaction
2. Integrated rate method:

- a. Acid hydrolysis of methyl acetate with hydrochloric acid.
- b. Saponification of ethyl acetate.
- c. Compare the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate

Reference Books:

1. A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall,
2. A.I. Vogel, Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
3. B.D.Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

CORE COURSE PHYSICS-2
(Theory-04 Credits, Practicals -02 Credits)

WAVES AND OPTICS

Superposition of Two Collinear Harmonic oscillations: Linearity and Superposition Principle. (1) Oscillations having equal frequencies and (2) Oscillations having different frequencies (Beats). (4 Lectures)

Superposition of Two Perpendicular Harmonic Oscillations: Graphical and Analytical Methods. Lissajous Figures (1:1 and 1:2) and their uses. (2 Lectures)

Waves Motion- General: Transverse waves on a string. Travelling and standing waves on a string. Normal Modes of a string. Group velocity, Phase velocity. Plane waves. Spherical waves, Wave intensity. (7 Lectures)

Fluids: Surface Tension: Synclastic and anticlastic surface - Excess of pressure - Application to spherical and cylindrical drops and bubbles - variation of surface tension with temperature - Jaeger's method. Viscosity: Viscosity - Rate flow of liquid in a capillary tube - Poiseuille's formula - Determination of coefficient of viscosity of a liquid - Variations of viscosity of a liquid with temperature lubrication. Physics of low pressure - production and measurement of low pressure - Rotary pump - Diffusion pump - Molecular pump - Knudsen absolute gauge - penning and pirani gauge - Detection of leakage. (6 Lectures)

Sound: Simple harmonic motion - forced vibrations and resonance - Fourier's Theorem - Application to saw tooth wave and square wave - Intensity and loudness of sound - Decibels - Intensity levels - musical notes - musical scale. Acoustics of buildings: Reverberation and time of reverberation - Absorption coefficient - Sabine's formula - measurement of reverberation time - Acoustic aspects of halls and auditoria. (6 Lectures)

Wave Optics: Electromagnetic nature of light. Definition and Properties of wave front. Huygens Principle. (3 Lectures)

Interference: Interference: Division of amplitude and division of wave front. Young's Double Slit experiment. Lloyd's Mirror and Fresnel's Biprism. Phase change on reflection: Stokes' treatment. Interference in Thin Films: parallel and wedge-shaped films. Fringes of equal inclination (Haidinger Fringes); Fringes of equal thickness (Fizeau Fringes). Newton's Rings: measurement of wavelength and refractive index. (10 Lectures)

Michelson's Interferometer: (1) Idea of form of fringes (no theory needed), (2) Determination of wavelength, (3) Wavelength difference, (4) Refractive index, (5) Visibility of fringes. (3 Lectures)

Diffraction: Fraunhofer diffraction: Single slit; Double Slit. Multiple slits & Diffraction grating. Fresnel Diffraction: Half-period zones. Zone plate. Fresnel Diffraction pattern of a straight edge, a slit and a wire using half-period zone analysis. (14 Lectures)

Polarization: Transverse nature of light waves. Plane polarized light - production and analysis. Circular and elliptical polarization. (5 Lectures)

Reference Books:

1. Fundamentals of Optics, F A Jenkins and H E White, 1976, McGraw-Hill
2. Principles of Optics, B.K. Mathur, 1995, Gopal Printing
3. Fundamentals of Optics, H.R. Gulati and D.R. Khanna, 1991, R. Chand Publication
4. University Physics. F.W. Sears, M.W. Zemansky and H.D. Young 13/e, 1986. Addison-Wesley

Physics Lab 2: Waves and Optics

60 Lectures

1. To investigate the motion of coupled oscillators
2. To determine the Frequency of an Electrically Maintained Tuning Fork by Melde's Experiment and to verify $\lambda^2 - T$ Law.
3. To study Lissajous Figures
4. Familiarization with Schuster's focussing; determination of angle of prism.
5. To determine the Coefficient of Viscosity of water by Capillary Flow Method (Poiseuille's method).
6. To determine the Refractive Index of the Material of a given Prism using Sodium Light.
7. To determine Dispersive Power of the Material of a given Prism using Mercury Light
8. To determine the value of Cauchy Constants of a material of a prism.
9. To determine the Resolving Power of a Prism.
10. To determine wavelength of sodium light using Fresnel Biprism.
11. To determine wavelength of sodium light using Newton's Rings.
12. To determine the wavelength of Laser light using Diffraction of Single Slit.
13. To determine wavelength of (1) Sodium & (2) Mercury light using plane diffraction Grating
14. To determine the Resolving Power of a Plane Diffraction Grating.
15. To measure the intensity using photo sensor and laser in diffraction patterns of single and double slits.

Reference Books:

1. Advanced Practical Physics for students, B.L.Flint & H.T.Worsnop, 1971, Asia Publishing House.
2. Advanced level Physics Practicals, Michael Nelson and Jon M. Osborn, 4th Edition, reprinted 1985, Heinemann Educational Publishers
3. A Text Book of Practical Physics, Indu Prakash and Ramakrishna, 11th Edition, 2011, Kitab Mahal, New Delhi.

DISCIPLINE SPECIFIC ELECTIVES - ANALYTICAL CHEMISTRY

(Select 2 Papers)

ANALYTICAL CHEMISTRY DSE -1

ANALYTICAL BIOCHEMISTRY

(Credits: Theory 04, Practicals 02)

SECTION I:

A. BASIC UNDERSTANDING OF THE STRUCTURES, PROPERTIES AND FUNCTIONS OF CARBOHYDRATES, LIPIDS, AND PROTEINS

1. Isolation and characterization of polysaccharides.
2. Classification of lipids, properties, functions and Biochemical functions of steroid hormones.
3. Proteins- structure, classification, isolation, characterization and functions Biochemistry of peptide hormones.
4. Enzymes- nomenclature, classification, effect of pH, temperature on enzyme activity, enzyme inhibition.
5. Lipoproteins

B. SECTION II .BIOCHEMISTRY OF DISEASE: A DIAGNOSTIC APPROACH

Clinical chemistry: a diagnostic approach by blood/urine analysis.

1. Blood: Composition and functions of blood, blood coagulation.
2. Blood collection and preservation of samples.
3. Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.
4. Formation of urine. Urine:
5. Collection and preservation of samples.
6. Composition and estimation of constituents of normal and pathological urine.

Analytical Chemistry DSE-1 Lab: Analytical Biochemistry

Identification and estimation of the following:

1. Carbohydrates – qualitative and quantitative.
2. Lipids – qualitative.
3. Determination of the iodine number of oil.
4. Determination of the saponification number of oil.
5. Determination of cholesterol using Liebermann- Burchard reaction.
6. Proteins – qualitative.
7. Isolation of protein.
8. Determination of protein by the Biuret reaction.
9. Determination of nucleic acids

Suggested Readings:

1. T.G.Cooper: Tool of Biochemistry.
2. Keith Wilson and John Walker: Practical Biochemistry.
3. Alan H Gowenlock: Varley's Practical Clinical Biochemistry.
4. Thomas M. Devlin: Textbook of Biochemistry.
5. Jeremy M. Berg, John L Tymoczko, Lubert Stryer: Biochemistry.
6. G. P. Talwar and M Srivastava: Textbook of Biochemistry and Human Biology.
7. A.L.Lehninger: Biochemistry.
8. O. Mikes, R.A. Chalmers: Laboratory Handbook of Chromatographic Methods.

DISCIPLINE SPECIFIC ELECTIVE-ANALYTICAL CHEMISTRY

ANALYTICAL CHEMISTRY DSE -2 INSTRUMENTAL METHODS OF ANALYSIS (Credits: Theory 04, Practicals 02)

Unit I. An Introduction to Spectroscopic Method of Analysis:

Unit II. UV AND Visible Spectrophotometry:

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

Unit III. IR Spectrophotometry:

- A. Principle
- B. Instrumentation
- C. applications: Identification of the functional groups and simple organic molecules.

Unit IV. Atomic Spectroscopy:

- A. Types
- B. Atomizer
- C. Atomic absorption and emission
- D. Applications

Unit V. ^1H NMR Spectroscopy:

- A. Principle
- B. Instrumentation
- C. Factors affecting chemical shift (Electronegativity, Anisotropy, etc.)
- D. Spin-spin coupling
- E. Coupling constant
- E. Applications: Deuterium exchange, effect of restricted rotation (e.g. DMF), identification of simple organic compounds using ^1H NMR spectra along with IR spectral data.

Analytical Chemistry DSE 2 Lab: Instrumental Methods of Analysis

1. Verification of Lambert-Beer's law using UV-Vis spectrophotometer for CuSO_4 solution.
2. Determination of the pK_a of an indicator (Phenolphthalein) using spectrophotometer.
3. To determine the isoelectric pH of a protein.
4. Identification of structure of simple organic compounds using IR- spectroscopy (IR spectra should be provided)
5. Synthesis of acetanilide and its characterisation using ^1H NMR and IR spectroscopy.
6. Synthesis of *m*-dinitro benzene and its characterisation using ^1H NMR and IR spectroscopy.
7. Isolation of DNA from onion and its characterisation using UV spectroscopy.

Suggested Readings:

1. P.W. Atkins: Physical Chemistry.
2. G.W. Castellan: Physical Chemistry.
3. C.N. Banwell: Fundamentals of Molecular Spectroscopy.
4. Brian Smith: Infra red Spectral Interpretations: A Systematic Approach.
5. W.J. Moore: Physical Chemistry

DISCIPLINE SPECIFIC ELECTIVE – ANALYTICAL CHEMISTRY

ANALYTICAL CHEMISTRY DSE- 3 GREEN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

(4 Lectures)

Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals – different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solvent less processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents, designing of biodegradable products; prevention of chemical accidents; strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

(24 Lectures)

Examples of Green Synthesis/ Reactions

1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, disodium iminodiacetate (alternative to Strecker synthesis), citral, ibuprofen, paracetamol, furfural.
2. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzoic acid), Oxidation (of toluene, alcohols). Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation. Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2-dihydrotriazine derivatives; benzimidazoles.
3. Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizzaro reaction, Strecker synthesis, Reformatsky reaction.
4. Selective methylation of active methylene group using dimethylcarbonate: Solid-state polymerization of amorphous polymers using diphenylcarbonate; Use of "Clayon", a nonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in organic syntheses; Biocatalysis in organic syntheses.

(24 Lectures)

Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solvent less reactions; oncovalent derivatization; Green chemistry in sustainable development.

(8 Lectures)

Reference Books:

1. V.K. Ahluwalia & M.R. Kidwai: *New Trends in Green Chemistry*, Anamalaya Publishers (2005).
2. P.T. Anastas & J.K. Warner: *Oxford Green Chemistry- Theory and Practical*, University Press (1998).
3. A.S. Maitland: *Introduction to Green Chemistry*, Marcel Dekker (2001).
4. M.C. Cann & M.E. Connely: *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).
5. M.A. Ryan & M. Tinnesand, *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).

Analytical Chemistry DSE 3 Lab: Green Chemistry

60 Lectures

1. Safer starting materials

The Vitamin C clock reaction using Vitamin C tablets, tincture of iodine, hydrogen peroxide and liquid laundry starch.

- a. Effect of concentration on clock reaction
- b. Effect of temperature on clock reaction. (if possible)

2. Using renewable resources

Preparation of biodiesel from vegetable oil.

3. Avoiding waste

Principle of atom economy.

Use of molecular model kit to simulate the reaction to investigate how the atom economy can illustrate Green Chemistry.

Preparation of propene by two methods can be studied

(I) Triethylamine ion + OH⁻ → propene + trimethylpropene + water

(II) 1-propanol + H₂SO₄ + Δ → propene + water

The other types of reactions, like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.

4. Use of enzymes as catalysts

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide
Alternative Green solvents.

5. Diels Alder reaction in water

Reaction between furan and maleic acid in water and at room temperature rather than in benzene and reflux.

6. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.

7. Mechanochemical solvent free synthesis of azomethines

8. Co-crystal controlled solid state synthesis (C2S3) of N-organophthalimide using phthalic anhydride and 3-aminobenzoic acid.

Alternative sources of energy

9. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).

10. Photo reduction of benzophenone to benzopinacol in the presence of sunlight.

Reference Books:

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

2. Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
3. Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
4. Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. *Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi*. Bangalore CISBN 978-93-81141-55-7 (2013).
5. Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society (2008).
6. Cann, M. C. & Thomas, P. *Real world cases in Green Chemistry*, American Chemical Society (2008).
7. Pavia, D. L. Lamponan, G. H. & Kriz, G.S. *WB Introduction to organic laboratory*

DISCIPLINE SPECIFIC ELECTIVES – ANALYTICAL CHEMISTRY

ANALYTICAL CHEMISTRY DSE 4 INDUSTRIAL CHEMICALS AND ENVIRONMENT (Credits: Theory-04, Practicals-02)

Industrial Gases and Inorganic Chemicals

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

Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

(10 Lectures)

Industrial Metallurgy

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

(4 Lectures)

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. Environmental effects of ozone, 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, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

Water Pollution: Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems.

Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal. Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

(30 Lectures)

Energy & Environment

Sources of energy: Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel, etc. Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.

(10 Lectures)

Biocatalysis

Introduction to Biocatalysis: Importance in “Green Chemistry” and Chemical Industry.

(6 Lectures)

Reference Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
3. J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.

4. S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
 5. K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
 6. S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
 7. S.E. Manahan, *Environmental Chemistry*, CRC Press (2005).
 8. G.T. Miller, *Environmental Science* 11th edition. Brooks/ Cole (2006).
 9. A. Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).
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Analytical Chemistry DSE 4 Lab: Industrial Chemicals & Environment

60 Lectures

1. Determination of dissolved oxygen in water.
2. Determination of Chemical Oxygen Demand (COD)
3. Determination of Biological Oxygen Demand (BOD)
4. Percentage of available chlorine in bleaching powder.
5. Measurement of chloride, sulphate and salinity of water samples by simple titration method (AgNO_3 and potassium chromate).
6. Estimation of total alkalinity of water samples (CO_3^{2-} , HCO_3^-) using double titration method.
7. Measurement of dissolved CO_2 .
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

Reference Books:

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

DISCIPLINE SPECIFIC ELECTIVES –CHEMISTRY

CHEMISTRY DSE-1

APPLICATIONS OF COMPUTERS IN CHEMISTRY (Credits: Theory-04, Practicals-02)

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++); Software Products (Office, chemsketch, scilab, matlab, hyperchem, etc.), internet application. (5 Lecture)

Use of Programming Language for solving problems in Chemistry

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

Programming Language – QBASIC; Commands: INPUT and PRINT

Commands; GOTO, If, ELSEIF, THEN and END IF Commands; FOR and NEXT Commands; 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 Commands.

Simple programs using above mentioned commands.

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

Solution of quadratic equation, polynomial equations (formula, iteration and Newton – Raphson methods, binary bisection and Regula Falsi); Numerical differential, Numerical integration (Trapezoidal rule), Simultaneous equations, Matrix addition and multiplication, Statistical analysis. (40 Lecture)

Use of Software Products

Computer Software like Scilab, Excel, etc to solve some of the plotting or calculation problems.

Basic idea of Molecular Modelling using software like chemsketch, arguslab and Accelrys JDraw etc for geometry optimization and potential energy surface (local and global minima) (15 lecture)

Chemistry DSE 1 Lab: Application of Computers in Chemistry

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. Matrix operations.
6. 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, etc.

Use of Software Products

1. Computer Software like Scilab and Excel, etc for data handling and manipulation.
2. Simple exercises using molecular visualization software like Chems sketch, Arguslab and Accelrys JDraw, geometry optimization and potential energy surface of molecules like carbon dioxide, water, ethane, cyclohexane and benzene (local and global minima)

Reference Books:

1. McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
2. Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005). Steiner, E. The Chemical Maths Book Oxford University Press (1996).
3. Yates, P. Chemical Calculations. 2nd Ed. CRC Press (2007).
4. Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5.
5. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001) 487 pages.
6. Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985).
7. Venit, S.M. Programming in BASIC: Problem solving with structure and style. Jaico Publishing House: Delhi (1996).

DISCIPLINE SPECIFIC ELECTIVE – CHEMISTRY

CHEMISTRY DSE-2 MOLECULAR MODELLING & DRUG DESIGN

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Introduction to Molecular Modelling:

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature. (10 Lectures)

Force Fields:

Fields. Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water. (14 Lectures)

Energy Minimization and Computer Simulation:

Minimization and related methods for exploring the energy surface. Non-derivative method, First and second order minimization methods. Computer simulation methods. Simple thermodynamic properties and Phase Space. Boundaries. Analyzing the results of a simulation and estimating Errors. (12 Lectures)

Molecular Dynamics & Monte Carlo Simulation:

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules. Models used in Monte Carlo simulations of polymers. (12 Lectures)

Structure Prediction and Drug Design:

Structure prediction - Introduction to comparative Modelling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design, Drug Discovery – Chemoinformatics – QSAR. (12 Lectures)

Reference Books:

1. A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
2. J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
3. Satya Prakash Gupta, QSAR and Molecular Modelling, Springer – Anamosa Publishers, 2008.

Chemistry DSE 2 Lab: Molecular Modelling & Drug Design

1. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
2. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerisation of *cis* and *trans* 2-butene.
3. Visualize the electron density and electrostatic potential maps for LiH, HF, N₂, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.

4. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
5. (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).
6. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
7. Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
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. (a) Compare the optimized bond angles H₂O, H₂S, H₂Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.
Note: Software: ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem, or any similar software.

Reference Books:

1. A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
2. J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
3. Satya Prakash Gupta, QSAR and Molecular Modelling, Springer - Anamaya Publishers, 2008.

DISCIPLINE SPECIFIC ELECTIVE – CHEMISTRY

DSE CHEMISTRY 3

NOVEL INORGANIC SOLIDS (Credits: Theory-04, Practicals-02)

Synthesis and modification of inorganic solids:

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods. (10 Lectures)

Inorganic solids of technological importance:

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments. One-dimensional metals, molecular magnets, inorganic liquid crystals.

(10 Lectures)

Nanomaterials:

Overview of nanostructures and nanomaterials: classification.

Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires.

Bioinorganic nanomaterials, DNA and nanomaterials, natural and antisical nanomaterials, bionanocomposites.

(10 Lectures)

Introduction to 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, super alloys thermoplastics, thermosets and composite materials.

(10 Lectures)

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, environmental effects on composites, applications of composites.

(10 Lectures)

Speciality polymers:

Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene and polypyrrole, applications of conducting polymers, Ion-exchange resins and their applications. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

(10 Lectures)

Reference Books:

1. Atkins, Peter, Overton, Tina, Rourke, Jonathan, Weller, Mark and Armstrong, Fraser *Shriver & Atkins' Inorganic Chemistry, 5th Edition*, Oxford University Press 2011-2012.
2. Adam, D.M. *Inorganic Solids: An introduction to concepts in solid-state structural chemistry*, John Wiley and Sons, London, New York, Sydney, Toronto, 1974
3. Poole Jr., Charles P., Owens, Frank J., *Introduction to Nanotechnology* John Wiley and Sons, 2003.

Chemistry DSE 3 Lab: Novel Inorganic Solids

1. Determination of cation exchange method
2. Determination of total difference of solids.
3. Synthesis of hydrogel by co-precipitation method.
4. Synthesis of silver and gold metal nanoparticles.

Reference Book: Fahlman, B.D., *Materials Chemistry*, Springer, 2007

DISCIPLINE SPECIFIC ELECTIVE – CHEMISTRY

DSE CHEMISTRY 4 POLYMER CHEMISTRY

(Credits: Theory-06, Practicals-02)

Theory: 60 Lectures

Introduction and history of polymeric materials:

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers. (4 Lectures)

Functionality and its importance:

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bifunctional systems, Poly-functional systems. (8 Lectures)

Kinetics of Polymerization:

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques. (8 Lectures)

Crystallization and crystallinity:

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

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

Determination of molecular weight of polymers (M_n , M_w , etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index. (8 Lectures)

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

Polymer Solution – Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures. (8 Lectures)

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

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly (vinyl chloride) and related polymers, poly (vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly (p-phenylene sulphide polypyrrole, polythiophene)]. (10 Lectures)

Reference Books:

1. *Seymour's Polymer Chemistry*, Marcel Dekker, Inc.
2. G. Odian: *Principles of Polymerization*, John Wiley.
3. F.W. Billmeyer: *Text Book of Polymer Science*, John Wiley.
4. P. Ghosh: *Polymer Science & Technology*, Tata McGraw-Hill.
5. R.W. Lenz: *Organic Chemistry of Synthetic High Polymers*.

Chemistry DSE 4 Lab: Polymer Chemistry

Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).
 - a. Purification of monomer
 - b. Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutyronitrile (AIBN)
2. Preparation of nylon 66/6. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
 - a. Preparation of IPC
 - b. Purification of IPC
 - c. Interfacial polymerization
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 by viscometry:
 - (a) Polyacrylamide-aq. NaNO₂ solution
 - (b) (Poly vinyl propylidene (PVP) in water
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: Polyethylene glycol (PEG) (OH Group).
4. Testing of mechanical properties of polymers.
5. Determination of hydroxyl number of a polymer using colorimetric method.

Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method
2. Instrumental Techniques
3. IR studies of polymers
4. DSC analysis of polymers
5. Preparation of polyacrylamide and its electrophoresis

*at least 7 experiments to be carried out.

Reference Books:

1. Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
2. Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
3. Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
4. Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
5. Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
6. L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)
7. Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)
8. Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013)

DISCIPLINE SPECIFIC ELECTIVE – CHEMISTRY

DSE CHEMISTRY 5 RESEARCH METHODOLOGY FOR CHEMISTRY (Credits: Theory-05, Tutorials-01)

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. (20 Lectures)

Methods of Scientific Research and Writing Scientific Papers:

Reporting practical and project work. 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, publications of scientific work. Writing ethics. Avoiding plagiarism.

(20 Lectures)

Chemical Safety and Ethical Handling of Chemicals:

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

(12 Lectures)

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.

(13 Lectures)

Electronics

Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers, typical circuits involving operational amplifiers for electrochemical instruments. Elementary aspects of digital electronics.

(10 Lectures)

Reference Books:

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2nd Ed. Prentice-Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
3. Topping, J. (1984) *Errors of observation and their treatment*. Fourth Ed., Chapman Hall, London.
4. Harris, D. C. *Quantitative chemical analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
5. Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*. Cambridge Univ. Press (2001) 487 pages.
6. Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992. OSU safety manual 1.01.

DISCIPLINE SPECIFIC ELECTIVE – CHEMISTRY

DSE CHEMISTRY 6 INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE (Credits: Theory-04, Practicals-02)

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, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

Ceramics: Brief introduction to types of ceramics. Superconducting and semiconducting oxides, fullerenes, carbon nanotubes and carbon fibre.

Cements: Manufacture of cement and the setting process, quick setting cements.

(16 Lectures)

Fertilizers:

Different types of fertilizers (N, P and K). Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates, superphosphate of lime.

(8 Lectures)

Surface Coatings:

Brief introduction to and classification of surface coatings. Paints and pigments - formulation, composition and related properties. Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

(4 Lectures)

Batteries:

Working of the following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.

(10 Lectures)

Catalysis:

General principles and properties of catalysts, homogenous catalysis (catalytic steps and examples) and heterogeneous catalysis (catalytic steps and examples) and their industrial applications, Deactivation or regeneration of catalysts.

Application of zeolites as catalysts.

(6 Lectures)

Chemical explosives:

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

(6 Lectures)

Reference Books:

1. Stocchi, E., *Industrial Chemistry*, Vol I, Ellis Horwood Ltd. UK, 1990
2. Felder, R. M. and Rousseau, R. W., *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi, 2005.
3. Kingery, W. D., Bowen H. K. and Uhlmann, D. R. *Introduction to Ceramics*, Wiley Publishers, New Delhi, 1976.
4. Kent, J. A. (ed) *Riegel's Handbook of Industrial Chemistry*, 9th Ed., CBS Publishers, New Delhi, 1997
5. Jain, P. C. and Jain, M. *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi 2005
6. Gopalan, R., Venkappayya, D. and Nagarajan, S. *Engineering Chemistry*, Vikas Publications, New Delhi, 2004.
7. Sharma, B. K. *Engineering Chemistry*, Goel Publishing House, Meerut, 2006

Chemistry DSE 6 Lab: Inorganic Materials of Industrial Importance

1. Determination of free acidity in ammonium sulphate fertilizer.
2. Estimation of Calcium in Calcium ammonium nitrate fertilizer.
3. Estimation of phosphoric acid in superphosphate fertilizer.
4. Electroless metallic coatings on ceramic and plastic material.
5. Determination of composition of dolomite (by complexometric titration).
6. Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
7. Analysis of Cement.
8. Preparation of pigment (zinc oxide).

Reference Books:

1. Stocchi, E., *Industrial Chemistry*, Vol I, Ellis Horwood Ltd. UK, 1990
2. Felder, R. M. and Rousseau, R.W., *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi, 2005.
3. Kingery, W. D., Bowen H. K. and Uhlmann, D. R. *Introduction to Ceramics*, Wiley Publishers, New Delhi, 1976.
4. Kent, J. A. (ed) *Riegel's Handbook of Industrial Chemistry, 9th Ed.*, CBS Publishers, New Delhi, 1997
5. Jain, P. C. and Jain, M. *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
6. Gopalan, R., Venkappayya, D. and Nagarajan, S. *Engineering Chemistry*, Vikas Publications, New Delhi, 2004.
7. Sharma, B. K. *Engineering Chemistry*, Goel Publishing House, Meerut, 2006

DISCIPLINE SPECIFIC ELECTIVE – CHEMISTRY

DSE CHEMISTRY 7 CHEMISTRY OF d-BLOCKELEMENTS, QUANTUM CHEMISTRY & SPECTROSCOPY (Compulsory) (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Section A: Inorganic Chemistry-3 (30 Lectures)

Transition Elements (3d series)

General group trends with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties, ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu.

Lanthanides and actinides: Electronic configurations, oxidation states, colour, magnetic Properties, lanthanide contraction, separation of lanthanides (ion exchange method only).

(12 Lectures)

Coordination Chemistry

Valence Bond Theory (VBT): Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT. IUPAC system of nomenclature.

(8 Lectures)

Crystal Field Theory

Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of D. Spectrochemical series. Comparison of CFSE for *Oh* and *Td* complexes, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, Square planar coordination.

(10 Lectures)

Section B: Physical Chemistry-4 (30 Lectures)

Quantum Chemistry & 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. 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.

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

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

(24 Lectures)

Photochemistry

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

(6 Lectures)

Reference Books:

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

Chemistry DSE 7 Lab: Chemistry of d-Block Elements, Quantum Chemistry & Spectroscopy

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 $CuSO_4/KMnO_4/K_2Cr_2O_7$ in a solution of unknown concentration
2. Analyse the given vibration-rotation spectrum of $HCl(g)$

Reference Books:

1. A.I. Vogel, *Qualitative Inorganic Analysis*, Prentice Hall, 7th Edn.
2. A.I. Vogel, *Quantitative Chemical Analysis*, Prentice Hall, 6th Edn.
3. B.D. Khosla, *Senior Practical Physical Chemistry*, R. Chand & Co.

DISCIPLINE SPECIFIC ELECTIVE – CHEMISTRY

DSE CHEMISTRY 8 ORGANOMETALLICS, BIOINORGANIC CHEMISTRY, POLYNUCLEAR HYDROCARBONS AND UV, IR SPECTROSCOPY (Credits: Theory-04, Practicals-02)

Section A: Inorganic Chemistry-4 (30 Lectures)

Chemistry of 3d metals, Oxidation states displayed by Cr, Fe, Co, Ni and Co.

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

Peroxo compounds of Cr, $K_2Cr_2O_7$, $KMnO_4$, $K_4[Fe(CN)_6]$, $K_3[Fe(CN)_6]$, sodium nitroprusside, $[Co(NH_3)_6]Cl_3$, $Na_3[Co(NO_2)_6]$. (6 Lectures)

Organometallics Compounds

Definition and Classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeise's salt and ferrocene. EAN rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals. p-acceptor behaviour of carbon monoxide. Synergic effects (VB approach) - (MO diagram of CO can be referred to for synergic effect to IR frequencies). (12 Lectures)

Bio-Inorganic Chemistry

A brief introduction to bio-inorganic chemistry. Role of metal ions present in biological systems with special reference to Na, K and Mg ions: Na/K pump; Role of Mg ions in energy production and chlorophyll. Role of iron in oxygen transport, haemoglobin, myoglobin, storage and transport of iron. (12 Lectures)

Section B: Organic Chemistry-4 (30 Lectures)

Polynuclear and heteronuclear aromatic compounds:

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

Active methylene compounds:

Preparation: Claisen ester condensation. Keto-enol tautomerism.

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

Application of Spectroscopy to Simple Organic Molecules. Application of visible, ultraviolet and infrared spectroscopy in organic molecules. Electromagnetic radiations, electronic transitions, λ_{max} & ϵ_{max} , chromophore, auxochrome, bathochromic and hypsochromic shifts. Application of electronic spectroscopy and Woodward rules for calculating λ_{max} of conjugated dienes and α,β - unsaturated compounds. Infrared radiation and types of molecular vibrations, functional group and fingerprint region. IR spectra of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on $>C=O$ stretching absorptions). (12 Lectures)

Reference Books:

1. James E. Huheey, Ellen Keiter & Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
2. G.L. Miessler & Donald A. Tarr: *Inorganic Chemistry*, Pearson Publication.
3. J.D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.

4. F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley & Sons.
5. I.L. Finar: *Organic Chemistry* (Vol. I & II), E.L.B.S.
6. John R. Dyer: *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall.
7. R.M. Silverstein, G.C. Bassler & T.C. Morrill: *Spectroscopic Identification of Organic Compounds*, John Wiley & Sons.
8. R.T. Morrison & R.N. Boyd: *Organic Chemistry*, Prentice Hall.
9. Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
10. Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand.

Chemistry DSE 8 Lab: Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons and UV, IR Spectroscopy

Section A: Inorganic Chemistry

1. Separation of mixtures by chromatography: Measure the R_f (Combination of two ions to be given) value in each case. ii) Paper chromatographic separation of Ni^{2+} , Co^{2+} , Mn^{2+} and Zn^{2+}
2. Preparation of any two of the following complexes and measurement of their conductivity: (i) tetraamminecarbonatocobalt (III) nitrate (ii) tetraamminecopper (II) sulphate (iii) potassium trioxalatoferrate (III) trihydrate. Compare the conductance of the complexes with that of M/1000 solution of NaCl, $MgCl_2$ and $LiCl_3$.

Section B: Organic Chemistry

1. Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (-COOH, alcoholic, phenolic, carbohydrates, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

Reference Books:

1. A.I. Vogel: *Qualitative Inorganic Analysis*, Prentice Hall, 7th Edn.
2. A.I. Vogel: *Quantitative Chemical Analysis*, Prentice Hall, 6th Edn.
3. A.I. Vogel: *Textbook of Practical Organic Chemistry*, Prentice Hall, 5th Edn.
4. F. G. Mann & B. C. Saunders: *Practical Organic Chemistry*, Orient Longman (1960).

DISCIPLINE SPECIFIC ELECTIVE – CHEMISTRY

DSE CHEMISTRY 9 MOLECULES OF LIFE (Credits: Theory-04, Practicals-02)

Unit 1: Carbohydrates (10 Lectures)

Classification of carbohydrates, reducing and non reducing sugars, General Properties of Glucose and Fructose, their open chain structure. Epimers, mutarotation and anomers. Determination of configuration of Glucose (Fischer proof). Cyclic structure of glucose. Haworth projections. Cyclic structure of fructose. Linkage between monosaccharides, structure of disaccharides (sucrose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

Unit 2: Amino Acids, Peptides and Proteins (12 Lectures)

Classification of *Amino Acids*, Zwitterion structure and Isoelectric point. Overview of Primary, Secondary, Tertiary and Quaternary structure of proteins. Determination of primary structure of peptides, determination of N-terminal amino acid (by DNFB and Edman method) and C-terminal amino acid (by thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (tbutyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid phase synthesis.

Unit 3: Enzymes and Correlation with Drugs (10 Lectures)

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,

Unit 4: Nucleic Acids (10 Lectures)

Components of Nucleic acids: Adenine, guanine, thymine and Cytosine (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), Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation.

Unit 5: Lipids (8 Lectures)

Introduction to lipids, classification. Oils and fats: Common fatty acids present in oils and fats, Omega fatty acids, Trans fats, Hydrogenation, Saponification value, Iodine number. Biological importance of triglycerides, phospholipids, glycolipids, and steroids (cholesterol).

Unit 6: Concept of Energy in Biosystems (8 Lectures)

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, Krebs Cycle. Overview of catabolic pathways of Fats and Proteins. Interrelationships in the metabolic pathways of Proteins, Fats and Carbohydrates.

Reference Book:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Finar, I. L. *Organic Chemistry (Volume 2)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Biochemistry 7th Ed.*, W. H. Freeman.
5. Berg, J. M., Tymoczko, J. L. & Stryer, L. *Biochemistry 7th Ed.*, W. H. Freeman.

Chemistry DSE 9 Lab: Molecules of life

1. Separation of amino acids by paper chromatography
2. To determine the concentration of glycine solution by formylation method.
3. Study of titration curve of glycine
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. Differentiate between a reducing/ nonreducing sugar.
9. Extraction of DNA from onion/cauliflower
10. To synthesize aspirin by acetylation of salicylic acid and compare it with the ingredient of An aspirin tablet by TLC.

Reference Books:

1. Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. *Vogel's*
2. *Textbook of Practical Organic Chemistry*, ELBS.
Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.

**DISCIPLINE SELECTIVE ELECTIVE – MATHO-PHYSICS
DSE-PHYSICS**

**PHYSICS-DSC 1: ELECTRICITY AND MAGNETISM
(Credits: Theory-04, Practicals-02)**

Vector Analysis: Scalar and Vector product, gradient, divergence, Curl and their significance, Vector Integration, Line, surface and volume integrals of Vector fields, Gauss-divergence theorem and Stoke's theorem of vectors (statement only).

(12 Lectures)

Electrostatics: Electrostatic Field, electric flux, Gauss's theorem of electrostatics. Applications of Gauss theorem- Electric field due to point charge, infinite line of charge, uniformly charged spherical shell and solid sphere, plane charged sheet, charged conductor. Electric potential as line integral of electric field, potential due to a point charge, electric dipole, uniformly charged spherical shell and solid sphere. Calculation of electric field from potential. Capacitance of an isolated spherical conductor. Parallel plate, spherical and cylindrical condenser. Energy per unit volume in electrostatic field. Dielectric medium, Polarisation, Displacement vector. Gauss's theorem in dielectrics. Parallel plate capacitor completely filled with dielectric.

(22 Lectures)

Magnetism:

Magnetostatics: Biot-Savart's law & its applications- straight conductor, circular coil, solenoid carrying current. Divergence and curl of magnetic field. Magnetic vector potential. Ampere's circuital law.

Magnetic properties of materials: Magnetic intensity, magnetic induction, permeability, magnetic susceptibility. Brief introduction of dia-, para- and ferro-magnetic materials.

(10 Lectures)

Electromagnetic Induction: Faraday's laws of electromagnetic induction, Lenz's law, self and mutual inductance, L of single coil, M of two coils. Energy stored in magnetic field.

(6 Lectures)

Maxwell's equations and Electromagnetic wave propagation: Equation of continuity of current, Displacement current, Maxwell's equations, Poynting vector, energy density in electromagnetic field, electromagnetic wave propagation through vacuum and isotropic dielectric medium, transverse nature of EM waves, polarization.

(10 Lectures)

Reference Books:

1. Electricity and Magnetism, Edward M. Purcell, 1986, McGraw-Hill Education.
2. Electricity and Magnetism, J.H. Fewkes & J. Yarwood. Vol. I, 1991, Oxford Univ. Press.
3. Electricity and Magnetism, D C Tayal, 1988, Himalaya Publishing House.
4. University Physics, Ronald Lane Reese, 2003, Thomson Brooks/Cole.
5. D.J. Griffiths, Introduction to Electrodynamics, 3rd Edn, 1998, Benjamin Cummings.

Physics DSC 1 Lab: ELECTRICITY AND MAGNETISM

1. To use a Multimeter for measuring (a) Resistances, (b) AC and DC Voltages, (c) DC Current and (d) checking electrical fuses.
2. Ballistic Galvanometer:

3. Measurement of charge and current sensitivity
 - i. Measurement of CDR
 - ii. Determine a high resistance by Leakage Method
 - iii. To determine Self Inductance of a Coil by Rayleigh's Method.
4. To compare capacitances using De'Sauty's bridge.
5. Measurement of field strength B and its variation in a Solenoid (Determine dB/dx).
6. To study the Characteristics of a Series RC Circuit.
7. To study the a series LCR circuit and determine its (a) Resonant Frequency, (b) Quality Factor
8. To study a parallel LCR circuit and determine it's (a) Anti-resonant frequency and (b) Quality factor Q
9. To determine a Low Resistance by Carey Foster's Bridge.
10. To verify the Thevenin and Norton theorem
11. To verify the Superposition, and Maximum Power Transfer Theorem

Reference Books

1. Advanced Practical Physics for students, B.L.Flint & H.T.Worsnop, 1971, Asia Publishing House.
2. A Text Book of Practical Physics, Indu Prakash and Ramakrishna, 11th Edition, 2011, Kitab Mahal, New Delhi.
3. Advanced level Physics Practicals, Michael Nelson and Jon M. Osborn, 4th Edition, reprinted 1985, Heinemann Educational Publishers

DISCIPLINE SELECTIVE ELECTIVE – MATHO-PHYSICS

PHYSICS- DSE 2: ELEMENTS OF MODERN PHYSICS

(Credits: Theory-04, Practicals-02)

Planck's quantum, Planck's constant and light as a collection of photons; Photo-electric effect and Compton scattering. De Broglie wavelength and matter waves; Davisson-Germer experiment. (8 Lectures)

Problems with Rutherford model- instability of atoms and observation of discrete atomic spectra; Bohr's quantization rule and atomic stability; calculation of energy levels for hydrogen like atoms and their spectra. (4 Lectures)

Position measurement- gamma ray microscope thought experiment; Wave-particle duality, Heisenberg uncertainty principle- impossibility of a particle following a trajectory; Estimating minimum energy of a confined particle using uncertainty principle; Energy-time uncertainty principle. (4 Lectures)

Two slit interference experiment with photons, atoms and particles; linear superposition principle as a consequence; Matter waves and wave amplitude; Schrodinger equation for non-relativistic particles; Momentum and Energy operators; stationary states; physical interpretation of wave function, probabilities and normalization; Probability and probability current densities in one dimension (11 Lectures)

One dimensional infinitely rigid box- energy eigen values and eigen functions, normalization; Quantum dot as an example; Quantum mechanical scattering and tunnelling in one dimension - across a step potential and across a rectangular potential barrier. (12 Lectures)

Size and structure of atomic nucleus and its relation with atomic weight; Impossibility of an electron being in the nucleus as a consequence of the uncertainty principle. Nature of nuclear force, NZ graph, semi-empirical mass formula and binding energy. (6 Lectures)

Radioactivity: stability of nucleus; Law of radioactive decay; Mean life & half-life; α decay; β decay - energy released, spectrum and Pauli's prediction of neutrino; γ -ray emission. (11 Lectures)

Fission and fusion - mass deficit, relativity and generation of energy; Fission - nature of fragments and emission of neutrons. Nuclear reactor: slow neutrons interacting with Uranium 235; Fusion and thermonuclear reactions. (4 Lectures)

Reference Books:

1. Concepts of Modern Physics, Arthur Beiser, 2009, McGraw-Hill
2. Modern Physics, John R. Taylor, Chris D. Zafiratos, Michael A. Dubson, 2009, PHI Learning
3. Six Ideas that Shaped Physics: Particle Behave like Waves, Thomas A. Moore, 2003, McGraw Hill
4. Quantum Physics, Berkeley Physics Course Vol.4. E.H. Wichman, 2008, Tata McGraw-Hill Co.
5. Modern Physics, R.A. Serway, C.J. Moses, and C.A. Moyer, 2005, Cengage Learning

Physics-DSE 2 LAB: ELEMENTS OF MODERN PHYSICS

1. To determine value of Boltzmann constant using V-I characteristic of PN diode.
2. To determine work function of material of filament of directly heated vacuum diode.
3. To determine value of Planck's constant using LEDs of at least 4 different colours.
4. To determine the ionization potential of mercury.
5. To determine the wavelength of H-alpha emission line of Hydrogen atom.
6. To determine the absorption lines in the rotational spectrum of Iodine vapour.
7. To study the diffraction patterns of single and double slits using laser source and measure its intensity variation using Photo sensor and compare with incoherent source – Na light.
8. Photo-electric effect: photo current versus intensity and wavelength of light; maximum energy of photo-electrons versus frequency of light
9. To determine the value of e/m by magnetic focusing.
10. To setup the Millikan oil drop apparatus and determine the charge of an electron.
- 11.

Reference Books:

1. Advanced Practical Physics for students, B.L.Flint & H.T.Worsnop, 1971, Asia Publishing House.
2. Advanced level Physics Practicals, Michael Nelson and Jon M. Osborn, 4th Edition, reprinted 1985, Heinemann Educational Publishers
3. A Text Book of Practical Physics, Indu Prakash and Ramakrishna, 11th Edition, 2011, Kitab Mahal, New Delhi.

DISCIPLINE SELECTIVE ELECTIVE – MATHO-PHYSICS

PHYSICS-DSE 3: MEDICAL PHYSICS

(Theory-04, Practicals-02)

PHYSICS OF THE BODY-I

Mechanics of the body: Skeleton, forces, and body stability. Muscles and the dynamics of body movement
Physics of body crashing;
Energy household of the body: Energy balance in the body, Energy consumption of the body, Heat losses of the body, Pressure system of the body: Physics of breathing, Physics of the cardiovascular system

(10 Lectures)

PHYSICS OF THE BODY-II

Acoustics of the body: Nature and characteristics of sound, Production of speech, Physics of the ear, Diagnostics with sound and ultrasound

Optical system of the body: Physics of the eye.

Electrical system of the body: Physics of the nervous system, Electrical signals and information transfer.

(10 Lectures)

PHYSICS OF DIAGNOSTIC AND THERAPEUTIC SYSTEMS-I X-RAYS:

Electromagnetic spectrum – production of x-rays – x-ray spectra- Brehmsstrahlung- Characteristic x-ray – X-ray tubes – Coolidge tube – x-ray tube design – tube cooling stationary mode – Rotating anode x-ray tube – Tube rating – quality and intensity of x-ray. X-ray generator circuits – half wave and full wave rectification – filament circuit – kilo voltage circuit – high frequency generator – exposure timer – HT cables.

(7 Lectures)

RADIATION PHYSICS: Radiation units - exposure - absorbed dose – units: rad, gray - relative biological effectiveness - effective dose - inverse square law - interaction of radiation with matter - linear attenuation coefficient. Radiation Detectors -Thimble chamber- condenser chambers – Geiger counter – Scintillation counter – ionization chamber – Dosimeters – survey methods – area monitors – TLD and semiconductor detectors.

(7 Lectures)

MEDICAL IMAGING PHYSICS: X-ray diagnostics and imaging, Physics of nuclear magnetic resonance (NMR) – NMR imaging – MRI Radiological imaging – Radiography – Filters – grids – cassette – X-ray film – film processing – fluoroscopy – computed tomography scanner – principle function – display – generations – mammography. Ultrasound imaging – magnetic resonance imaging – thyroid uptake system – Gamma camera (Only Principle, function and display).

(9 Lectures)

RADIATION THERAPY PHYSICS: Radiotherapy – kilo voltage machines – deep therapy machines – Telecobalt machines – Medical linear accelerator. Basics of Teletherapy units – deep x-ray, Telecobalt units, medical linear accelerator – Radiation protection – external beam characteristics – phantom – dose maximum and build up – bolus – percentage depth dose – tissue – air ratio – back scatter factor.

(6 Lectures)

RADIATION AND RADIATION PROTECTION: Principles of radiation protection – protective materials-radiation effects – somatic, genetic stochastic & deterministic effect, Personal monitoring devices – TLD film badge – pocket dosimeter. Radiation dosimetry, Natural radioactivity, Biological effects of radiation, Radiation monitors.

(6 Lectures)

PHYSICS OF DIAGNOSTIC AND THERAPEUTIC SYSTEMS-II

Diagnostic nuclear medicine: Radiopharmaceuticals for radioisotope imaging, Radioisotope imaging equipment, Single photon and positron emission tomography
Therapeutic nuclear medicine: Interaction between radiation and matter Dose and isodose in radiation treatment.

(5 Lectures)

References:

1. Medical Physics, J.R. Cameron and J.G.Skofronick, Wiley (1978)
2. Basic Radiological Physics Dr. K. Thayalan - Jayapee Brothers Medical Publishing Pvt. Ltd. New Delhi (2003)
3. Christensen's Physics of Diagnostic Radiology: Curry, Dowdey and Murry - Lippincot Williams and Wilkins (1990)
4. Physics of Radiation Therapy : F M Khan - Williams and Wilkins, Third edition (2003)
5. Physics of the human body, Irving P. Herman, Springer (2007).
6. The essential physics of Medical Imaging: Bushberg, Seibert, Leidholdt and Boone Lippincot Williams and Wilkins, Second Edition (2002)
7. The Physics of Radiology-H E Johns and Cunningham.

Physics-DSE Lab 3: Medical Physics

1. Understanding the working of a manual Hg Blood Pressure monitor and measure the Blood Pressure.
2. Understanding the working of a manual optical eye-testing machine and to learn eye testing.
3. Correction of Myopia (short sightedness) using a combination of lenses on an optical bench/breadboard.
4. Correction of Hypermetropia/Hyperopia (long sightedness) using a combination of lenses on an optical bench/breadboard.
5. To learn working of Thermo luminescent dosimeter (TLD) badges and measure the background radiation.
6. Familiarization with Geiger-Muller (GM) Counter and to measure background radiation.
7. Familiarization with Radiation meter and to measure background radiation.
8. Familiarization with the construction of speaker-receiver system and to design a speaker-receiver system of given specification.

References:

1. Basic Radiological Physics Dr. K. Thayalan - Jayapee Brothers Medical Publishing Pvt. Ltd. New Delhi (2003)
2. Christensen's Physics of Diagnostic Radiology: Curry, Dowdey and Murry - Lippincot Williams and Wilkins (1990)
3. Physics of Radiation Therapy: F M Khan - Williams and Wilkins, Third edition (2003)
4. The essential physics of Medical Imaging: Bushberg, Seibert, Leidholdt and Boone Lippincot Williams and Wilkins, Second Edition (2002)
5. The Physics of Radiology-H E Johns and Cunningham.
6. Advanced Practical Physics for students, B.L.Flint & H.T.Worsnop, 1971, Asia Publishing House.
7. A Text Book of Practical Physics, Indu Prakash and Ramakrishna, 11th Edition, 2011, Kitab Mahal, New Delhi.

DISCIPLINE SELECTIVE ELECTIVE – MATHO-PHYSICS

DISCIPLINE SPECIFIC ELECTIVE – MATHEMATICS DSE- 1 MATHEMATICS

DIFFERENTIAL EQUATIONS

Ordinary Differential equations First order exact differential equations. Integrating factors, rules to find and integrating factor. First order higher degree equations solvable for $x, y, p=dy/dx$. Methods for solving higher-order differential equations. Basic theory of linear differential equations, Wronskian, and its properties. Solving an differential equation by reducing its order. Linear homogenous equations with constant coefficients. Linear non-homogenous equations. The method of variation of parameters, The Cauchy-Euler equation. Simultaneous differential equations, total differential equations.

Partial Differential Equations Order and degree of partial differential equations. Concept of linear and nonlinear partial differential equations. Formation of first order partial differential equations. Linear partial differential equation of first order, Lagrange's method, Charpit's method. Classification of second order partial differential equations into elliptic, parabolic and hyperbolic through illustrations only.

Recommended Books

1. Shepley L. Ross: Differential equations, Third edition, John Wiley and Sons, 1984
2. I. Sneddon: Elements of partial differential equations, McGraw-Hill, International Edition, 1967

DSE- 2 MATHEMATICS

CALCULUS AND GEOMETRY

Unit I: Calculus Limit and continuity of a function: (ϵ - δ and sequential approach). Properties of continuous functions including intermediate value theorem, Differentiability, Rolle's theorem, Lagrange's mean value theorem, Cauchy mean value theorem with geometrical interpretations. Uniform continuity. Definitions and techniques for finding asymptotes singular points, Tracing of standard curves. Integration of irrational functions. Reduction formulae. Rectification. Quadrature. Volumes.

Unit II: Geometry and Vector Calculus Techniques for sketching parabola, ellipse and hyperbola. Reflection properties of parabola, ellipse and hyperbola. Classification of quadratic equations representing lines, parabola, ellipse and hyperbola. Differentiation of vector valued functions, gradient, divergence, curl and their geometrical interpretation. Spheres, Cylindrical surfaces. Illustrations of graphing standard quadric surfaces like cone, ellipsoid.

Recommended Books

1. H. Anton, I. Bivens and S. Davis: Calculus, John Wiley and Sons (Asia) Pte. Ltd. 2002.
2. R.G. Bartle and D.R. Sherbert : Introduction to Real Analysis , John Wiley and Sons (Asia) Pte, Ltd; 1982

SKILL ENHANCEMENT COURSES

SEC -1

BIOTECHNOLOGY

(Credits 02)

The purpose of this course is to provide to the students of Science, a basic understanding of the principles, tools and techniques, and applications of the fast expanding fields of biotechnology. This would help the students to develop interactions/linkages with the industry and venture into Science entrepreneurship.

Unit I Biotechnology

Scope and Applications, Overview of Tools and Techniques.

Unit I Industrial Microbiology

Microbial resources for food, food additives, flavours, feed, single cell proteins, solvents, enzymes, organic acids, vitamins, pharmaceuticals, agrochemicals, bio-fertilizers. Waste decomposition and conversions, bio-fuels, Bioremediation, Recombinant proteins

Unit III Strain improvement

Screening, selection, mutation, recombination, protoplast fusion, DNA technology.

Unit IV Fermentation

Different types of fermentation – submerged and solid state; batch, fed batch and continuous; product-based – enzymes, alcohol, methane, acid, mixed acid and solvent. Types of fermenters-stirred tank, air lift fixed bed and fluidized. Downstream processing – filtration, centrifugation, extraction, chromatography, spray drying and lyophilisation.

Unit V Plant Biotechnology

Plant tissue culture and somatic cell genetics and their applications in agriculture, plant transformation-vectors and methods, genetic engineering and transgenic plants with useful agronomic traits and products.

Unit VI Animal Biotechnology

Cell culture and production of bio-products, gene manipulation and transgenic technology, gene therapy, vaccines, hybridoma technology and immunodiagnosics.

Unit VII Bio safety

Physical and Biological containment, environmental co-concerns.

Suggested Readings:

1. P.K. Gupta: Biotechnology and Genomics, Rastogi publishers (2003).
2. B.D. Singh: Biotechnology, Kalyani publishers, 1998 (Reprint 2001).
3. T.A. Brown: Gene cloning and DNA analysis: An Introduction, Blackwell Science (2001).
4. M.K. Razdan: Introduction to plant tissue culture, Oxford & IBH, New Delhi (2003).
5. Bernard R. Click & Jack J. Pasternak: Molecular Biotechnology, ASM Press, Washington (1998)

**SKILL ENHANCEMENT COURSE
SEC-2**

FORENSIC SCIENCE

Forensic Science pertains to analysis and examination of Physical evidence recovered from a crime scene to legal proceedings. Examinations of fingerprint, toxic substances detection of blood and other biological fluids, as well as examination of skeletal material, hair fiber etc is performed to provide scientific opinion for legal.

Unit I Definition, History, Development and Scope of Forensic Science. Divisions of Forensic Science and Laboratory Set up.

Unit II Basic Principles, theory and application of spectroscopy (U.V., I.R., Atomic Absorption Emission and Mass) and its forensic applications.

Unit III Electrophoresis (Immuno and Iso-electrofocusing) theory, principle and techniques. X-ray (Hard and Soft) techniques and their forensic applications.

Unit IV Forensic Chemistry: Introduction, Conventional methods of chemical analysis, presumptive tests (colour & spot); Drugs of Abuse:

Introduction and classification; Forensic Toxicology: Introduction and General methods of chemical analysis for alcohol, Classification of poisons.

Unit V Questioned documents: Definition, handwriting, characteristic, natural variation, comparison and forgery; Forensic photography – techniques and important of photography.

Unit VI Fingerprint Identification: History and development, biological basis of fingerprints, pattern types, scene of crime prints, methods of processing latent/fingerprints, ridge characteristics, comparison of fingerprints for establishing complete identity.

Unit VII Tool marks: their identification and importance in forensic science;

Trace evidence: Definition, identification and their importance in forensic science.

Unit VIII Identification and detection of biological fluids (Blood, Semen, Saliva and Urine) and their Medico-logical importance.

Unit IX Personal Identification through somatometry and Somatoscopy; Study and hair and fibers.

Unit X Examination of skeletal remains-identification of bones, differentiation between human and non human, determination of age, sex and height from skeletal remains.

Unit XI Modern Developments and their concepts (Nacre analysis, Brain fingerprinting, DNA Profiling, voice identification, Cyber crime, Odontology and Bitemarks).

Note; Practical demonstrations are compulsory as without the demonstration the students would not be able to understand the value of the specific topics of Forensic Science.

Practical demonstration of procedure of taking fingerprints; identification of pattern types, developing latent fingerprints (Powder Method), spot test for blood identification,

Somatoscopic observations, Age and Sex determination from skull, estimation of height from long bones, hair morphology, tests for fiber identification.

Suggested Readings

1. R. Saferstein: *Criminalistics*, Prentice Hall (1998).
2. B.R. Sharma: *Forensic Science in Criminal Investigation and Trials*, Central Law Agency, Allahabad (2003).
3. W.G. Eckert: *Introduction of Forensic Science*, CRE Press, Bock Raton (1997).
4. I.P. Singh and M.K. Bhasin: *A Laboratory Manual of Biological Anthropology*, K.R. Enterprises, N. Delhi (2005).
5. S. Nath: *An Introduction to Forensic Anthropology*, Gian Publishing House, N. Delhi (1989).
6. S. Nath: *Personal Identification through Fingerprints*, Shree Publisher & Distributors, New Delhi (2006)

**SKILL ENHANCEMENT COURSE
SEC-3**

GREEN METHODS IN CHEMISTRY (Credits: 02)

(Hands on Exercises: 60 Lectures)

Theory and Hands-on Experiments

Introduction: Definitions of Green Chemistry. Brief introduction of twelve principles of Green Chemistry, with examples, special emphasis on atom economy, reducing toxicity, green solvents,

Green Chemistry and catalysis and alternative sources of energy, Green energy and sustainability

The following Real world Cases in Green Chemistry should be discussed:

1. Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.
2. Designing of Environmentally safe marine antifoulant.
3. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
4. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.

SEC 3 Lab

1. Preparation and characterization of biodiesel from vegetable oil.
2. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.
3. Mechanochemical solvent free synthesis of azomethine.
4. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II)

Reference Books:

1. Anastas, P.T. and Warner, J.K. *Oxford Green Chemistry- Theory and Practical*, University Press, 1998
2. Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker, 2001
3. Cann, M.C. and Connely, M.E., *Real-World Cases in Green Chemistry*, American Chemical Society, Washington, 2000
4. Ryan, M.A. and Tinnesand, M., *Introduction to Green Chemistry*, American Chemical Society, Washington, 2002
5. Sharma, R.K., Sidhwani, I.T. and Chaudhari, M.K. *Green Chemistry Experiments: A monograph*, I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore ISBN 978-93-81141-55-7, 2013
6. Lancaster, Mike *Green Chemistry: An Introductory Text 2nd Ed.*, RSC Publishing, ISBN 978-1-84755-873-2, 2010
7. Wealth from waste: A green method to produce biodiesel from waste cooking oil

SKILL ENHANCEMENT COURSE
SEC-4
INTELLECTUAL PROPERTY RIGHTS (IPR)
(Credits: 02)

Theory: 30 Lectures

In this era of liberalization and globalization, the perception about science and its practices has undergone dramatic change. The importance of protecting the scientific discoveries, with commercial potential or the intellectual property rights is being discussed at all levels – statutory, administrative, and judicial. With India ratifying the WTO agreement, it has become obligatory on its part to follow a minimum acceptable standard for protection and enforcement of intellectual property rights. The purpose of this course is to apprise the students about the multifaceted dimensions of this issue.

Introduction to Intellectual Property:

Historical Perspective, Different Types of IP, Importance of protecting IP.

Copyrights

Introduction, How to obtain, Differences from Patents.

Trade Marks

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, Trade names, etc.

Differences from Designs.

Patents

Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Healthcare – balancing promoting innovation with public health, Software patents and their importance for India.

Geographical Indications

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Industrial Designs

Definition, How to obtain, features, International design registration.

Layout design of integrated circuits

Circuit Boards, Integrated Chips, Importance for electronic industry.

Trade Secrets

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

Different International agreements

(a) World Trade Organization (WTO):

(i) General Agreement on Tariffs & Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement (ii) General Agreement on Trade related Services (GATS) (iii) Madrid Protocol (iv) Berne Convention (v) Budapest Treaty

(b) Paris Convention

WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity

IP Infringement issue and enforcement – Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. Economic Value of Intellectual Property – Intangible assets and their valuation, Intellectual Property in the Indian Context – Various laws in India Licensing and technology transfer.

Reference Books:

1. Acharya: *Textbook on intellectual property rights*, Asia Law House (2001).
2. Guru & M.B. Rao, *Understanding Trips: Managing Knowledge in Developing Countries*, Sage Publications (2003).

**SKILL ENHANCEMENT COURSE
SEC-5**

BUSINESS SKILLS FOR CHEMISTS (Credits: 02)

Theory: 30 Lectures

Business Basics

Key business concepts: Business plans, market need, project management and routes to market.

Chemistry in Industry

Current challenges and opportunities for the chemistry-using industries, role of chemistry in India and global economies.

Making money

Financial aspects of business with case studies

Intellectual property

Concept of intellectual property, patents.

References:

www.rsc.org

**SKILL ENHANCEMENT COURSE
SEC-6**

FUEL CHEMISTRY (Credits: 02)

(Hands on Exercises: 60 Lectures)

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

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

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

Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels.

Petrochemicals:

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

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

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

Reference Books:

1. E. Stocchi: Industrial Chemistry, Vol -I, Ellis Horwood Ltd. UK.
2. P.C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
3. B.K. Sharma: Industrial Chemistry, Goel Publishing House, Meerut

**SKILL ENHANCEMENT COURSE
SEC-7**

PESTICIDE CHEMISTRY (Credits: 02)

(Hands on Exercises: 60 Lectures)

General introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship, synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,); Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

Practicals

1. To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
2. Preparation of simple organophosphates, phosphonates and thiophosphates

Reference Book:

1. R. Cremlyn: Pesticides, John Wiley.

**SKILL ENHANCEMENT COURSE
SEC-8**

CHEMOINFORMATICS (Credits: 02)

(Hands on Exercises: 60 Lectures)

Introduction to Chemoinformatics: History and evolution of chemoinformatics, Use of chemoinformatics,

Prospects of chemoinformatics, Molecular Modelling and Structure elucidation.

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.

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.

Applications: Prediction of Properties of Compounds; Linear Free Energy Relations;

Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modelling

Toxicity; Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer

Assisted Structure elucidations; Computer Assisted Synthesis Design, 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.

Hands-on Exercises

Reference Books:

1. Andrew R. Leach & Valerie, J. Gillet (2007) An introduction to Chemoinformatics. Springer: The Netherlands.

2. Gasteiger, J. & Engel, T. (2003) Chemoinformatics: A text-book. Wiley-VCH.
3. Gupta, S. P. (2011) QSAR & Molecular Modelling. Anamaya Pub.: New Delhi.