Proposed syllabus and Scheme of Examination

for

B.Sc. (Program) with Chemistry

Submitted

to

University Grants Commission

New Delhi

Under

Choice Based Credit System

April 2015
**Details of Courses Under Undergraduate Program (B.Sc.)**

<table>
<thead>
<tr>
<th>Course</th>
<th>*Credits</th>
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<tbody>
<tr>
<td><strong>I. Core Course</strong></td>
<td>**Theory+ Practical</td>
</tr>
<tr>
<td>(12 Papers)</td>
<td>12×4=48</td>
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<tr>
<td>04 Courses from each of the</td>
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<tr>
<td>03 disciplines of choice</td>
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<tr>
<td><strong>Core Course Practical / Tutorial</strong>*</td>
<td>12×2=24</td>
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<tr>
<td>(12 Practical/ Tutorials*)</td>
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<tr>
<td>04 Courses from each of the</td>
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<tr>
<td>03 Disciplines of choice</td>
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<td><strong>II. Elective Course</strong></td>
<td>6×4=24</td>
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<td>(6 Papers)</td>
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<td>Two papers from each discipline of choice</td>
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<td>including paper of interdisciplinary nature.</td>
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<tr>
<td><strong>Elective Course Practical / Tutorials</strong>*</td>
<td>6×2=12</td>
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<tr>
<td>(6 Practical / Tutorials*)</td>
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<tr>
<td>Two Papers from each discipline of choice</td>
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<td>including paper of interdisciplinary nature</td>
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<tr>
<td>• Optional Dissertation or project work in place of one Discipline elective paper (6 credits) in 6th Semester</td>
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</tbody>
</table>
III. Ability Enhancement Courses

1. Ability Enhancement Compulsory 
   \[2 \times 2 = 4\] 
   \[2 \times 2 = 4\] 
   (2 Papers of 2 credits each) 
   Environmental Science 
   English/MIL Communication

2. Skill Enhancement Course 
   \[4 \times 2 = 8\] 
   \[4 \times 2 = 8\] 
   (Skill Based) 
   (4 Papers of 2 credits each)

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

Proposed scheme for choice based credit system in B. Sc. Program

<table>
<thead>
<tr>
<th>CORE COURSE (12)</th>
<th>Ability Enhancement Compulsory Course (AECC) (2)</th>
<th>Skill Enhancement Course (SEC) (2)</th>
<th>Discipline Specific Elective DSE (6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I DSC- 1 A</td>
<td>Atomic Structure, Bonding, General Organic Chemistry &amp; Aliphatic</td>
<td>(English/MIL Communication)/Environmental Science</td>
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<td>Hydrocarbons</td>
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<td></td>
<td>DSC- 3 A</td>
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| II | DSC- 1 B    | Environmental Science (English/MIL Communication) |
|    | Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I |
|    | DSC- 3 B    |   |

| III | DSC- 1 C | SEC-1 |
|     | Solutions, Phase equilibrium, Conductance, Electrochemistry & Functional Group Organic Chemistry-II |
|     | DSC- 3 C |   |

<p>| IV | DSC- 1 D | SEC -2 |
|    | Chemistry of s- and p-block Elements, States of Matter &amp; Chemical |   |</p>
<table>
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<tr>
<th>Kinetics</th>
<th>DSC-3 D</th>
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<td>V</td>
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<td>SEC -3</td>
<td>DSE-1 A</td>
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<td>DSE-2 A</td>
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<td>VI</td>
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<td>DSE-3 B</td>
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<td>SEMESTER</td>
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<tr>
<td>I</td>
<td>Ability Enhancement Compulsory Course-I</td>
<td>English/MIL communications/ Environmental Science</td>
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<td></td>
<td>Core Course-I</td>
<td>DSC 1A</td>
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<td></td>
<td>Core Course-II</td>
<td>Atomic Structure, Bonding, General Organic Chemistry &amp; Aliphatic Hydrocarbons</td>
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<td>Core Course-II Practical/ Tutorial</td>
<td>Atomic Structure, Bonding, General Organic Chemistry &amp; Aliphatic Hydrocarbons Lab</td>
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<td>Core Course-III</td>
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<tr>
<td>II</td>
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<td>Core Course-IV</td>
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<td>Core Course-V</td>
<td>Chemical Energetics, Equilibria &amp; Functional Group Organic Chemistry-I</td>
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<td></td>
<td>Core Course-V Practical/ Tutorial</td>
<td>Chemical Energetics, Equilibria &amp; Functional Group Organic Chemistry-I Lab</td>
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<td>III</td>
<td>Core Course-VII</td>
<td>DSC 1C</td>
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<td>Core Course-VIII</td>
<td>Solutions, Phase Equilibria, Conductance, Electrochemistry &amp; Functional Group Organic Chemistry-II</td>
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<tr>
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<td>Core Course-VIII Practical/ Tutorial</td>
<td>Solutions, Phase Equilibria, Conductance, Electrochemistry &amp; Functional Group Organic Chemistry-II Lab.</td>
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<td>Core Course-IX</td>
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<td>IV</td>
<td>Core course-X</td>
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<td>Core Course-XI</td>
<td>Chemistry of s- and p-block elements, States of matter &amp; Chemical kinetics</td>
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<td>Course-XI Practical/Tutorial</td>
<td>Chemistry of s- and p-block elements, States of matter &amp; Chemical kinetics Lab</td>
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<td>Discipline Specific Elective -1</td>
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<td>Discipline Specific Elective-6</td>
<td>DSE-3B</td>
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<tr>
<td><strong>Total Credits</strong></td>
<td><strong>120</strong></td>
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**B.Sc. Program with Chemistry**

**Core papers Chemistry (Credit: 06 each) (CP 1-4):**

1. Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons (4) + Lab (4)
2. Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I (4) + Lab (4)
4. Chemistry of s- and p-block elements, States of matter and Chemical Kinetics (4) + Lab (4)

**Discipline Specific Elective papers (Credit: 06 each) (DSE 1, DSE 2): Choose 2**

**Chemistry**

1. Applications of Computers in Chemistry (4) + Lab (4)
2. Analytical Methods in Chemistry (4) + Lab (4)
3. Molecular Modelling & Drug Design (4) + Lab (4)
5. Polymer Chemistry (4) + Lab (4)
6. Research Methodology for Chemistry (5) + Tutorials (1)
7. Green Chemistry (4) + Lab (4)
8. Industrial Chemicals & Environment (4) + Lab (4)
9. Inorganic Materials of Industrial Importance (4) + Lab (4)
10. Instrumental Methods of Analysis (4) + Lab (4)
11. Chemistry of d-block elements, Quantum Chemistry and Spectroscopy (4) + Lab (4)
12. Organometallics, Bioinorganic chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy
13. Molecules of life (4) + Lab (4)
14. Dissertation

Note: Universities may include more options or delete some from this list

**Skill Enhancement Course (any four) (Credit: 02 each)- SEC 1 to SEC 4**
Chemistry
1. IT Skills for Chemists
2. Basic Analytical Chemistry
3. Chemical Technology & Society
4. Chemoinformatics
5. Business Skills for Chemists
6. Intellectual Property Rights
7. Analytical Clinical Biochemistry
8. Green Methods in Chemistry
9. Pharmaceutical Chemistry
10. Chemistry of Cosmetics & Perfumes
11. Pesticide Chemistry
12. Fuel Chemistry

Note: Universities may include more options or delete some from this list

Important:
1. Each University/Institute should provide a brief write-up about each paper outlining the salient features, utility, learning objectives and prerequisites.
2. University can add/delete some experiments of similar nature in the Laboratory papers.
3. University can add to the list of reference books given at the end of each paper.
CHEMISTRY-DSC 2A: ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS
(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

Section A: Inorganic Chemistry-I (30 Periods)


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

Rules for filling electrons in various orbitals, Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations.

(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


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.


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, oxymercuration-demercuration, Hydroboration-oxidation.
Alkynes: (Upto 5 Carbons) *Preparation:* Acetylene from CaC$_2$ 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 KMnO$_4$, ozonolysis and oxidation with hot alk. KMnO$_4$.

(12 Lectures)

Reference Books:
- J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
- Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand

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CHEMISTRY LAB: DSC 2A LAB: 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 KMnO$_4$.

3. Estimation of water of crystallization in Mohr’s salt by titrating with KMnO$_4$.

4. Estimation of Fe (II) ions by titrating it with K$_2$Cr$_2$O$_7$ using internal indicator.

5. Estimation of Cu (II) ions iodometrically using Na$_2$S$_2$O$_3$.

*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 Rf value in each case (combination of two compounds to be given)

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

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

Reference Books:

Semester II

CHEMISTRY-DSC 2B: CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY  
(Credits: Theory-04, Practicals-02)  
Theory: 60 Lectures

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 – Kirchhoff’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 $\Delta G$ and $\Delta G^\circ$, 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.


(8 Lectures)

**Alkyl and Aryl Halides**

**Alkyl Halides** (Upto 5 Carbons) Types of Nucleophilic Substitution ($S_N1$, $S_N2$ and $S_Ni$) reactions.

*Preparation*: from alkenes and alcohols.


**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: $\text{KNH}_2/\text{NH}_3$ (or $\text{NaNH}_2/\text{NH}_3$).

Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.
Alcohols, Phenols and Ethers (Upto 5 Carbons)

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


**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.


Reference Books:

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CHEMISTRY LAB- DSC 2B LAB: 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 (KNO₃, NH₄Cl).
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

- B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

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Semester III
CHEMISTRY-DSC 2C: SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY & FUNCTIONAL GROUP ORGANIC CHEMISTRY-II
(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

Section A: Physical Chemistry-2 (30 Lectures)

Solutions


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, FeCl₃-H₂O 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.


Electrochemistry

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 & reactions) to be studied in context to their structure.

**Carboxylic acids and their derivatives**

Carboxylic acids (aliphatic and aromatic)

*Preparation:* Acidic and Alkaline hydrolysis of esters.

*Reactions:* Hell – Vohlard - Zelinsky Reaction.

**Carboxylic acid derivatives (aliphatic):** (Upto 5 carbons)

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


(6 Lectures)

**Amines and Diazonium Salts**

Amines (Aliphatic and Aromatic): (Upto 5 carbons)

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


**Diazonium salts: Preparation:** from aromatic amines.

*Reactions:* conversion to benzene, phenol, dyes.

(6 Lectures)

**Amino Acids, Peptides and Proteins:**

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

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

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

(10 Lectures)

Carbohydrates: Classification, and General Properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, ascending and descending in monosaccharides. Structure of disacharrides (sucrose, cellobiose, maltose, lactose) and polysacharrides (starch and cellulose) excluding their structure elucidation.

(8 Lectures)

Reference Books:
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

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CHEMISTRY LAB-DSC 2C LAB: SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY & BIOMOLECULES

60 Lectures
Section A: Physical Chemistry

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

$$\text{I}_2(\text{aq}) + \text{I}^-(\text{aq}) \rightleftharpoons \text{I}_3^-(\text{aq})$$

$$\text{Cu}^{2+}(\text{aq}) + x\text{NH}_2(\text{aq}) \rightleftharpoons [\text{Cu(NH}_3]_x^{2+}$$

**Phase equilibria**

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

**Conductance**

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

**Potentiometry**

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

**Section B: Organic Chemistry**

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

II

1. Separation of amino acids by paper chromatography
2. Determination of the concentration of glycine solution by formylation method.
3. Titration curve of glycine
4. Action of salivary amylase on starch
5. Effect of temperature on the action of salivary amylase on starch.
6. Differentiation between a reducing/nonreducing sugar.

**Reference Books:**
CHEMISTRY-DSC 2D: CHEMISTRY OF S- AND P-BLOCK ELEMENTS, STATES OF MATTER & CHEMICAL KINETICS
(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

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, Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, Kroll process, Parting process, van Arkel-de Boer process and Mond’s process.

(s- and p-Block Elements)

Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electronegativity (Pauling, Mulliken, and 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

Hydrides and their classification (ionic, covalent and interstitial), structure and properties with respect to stability of hydrides of p-block elements.

Concept of multicentre bonding (diborane).

Structure, bonding and their important properties like oxidation/reduction, acidic/basic nature of the following compounds and their applications in industrial, organic and environmental chemistry.

Hydrides of nitrogen (NH$_3$, N$_2$H$_4$, N$_3$H, NH$_2$OH)
Oxoacids of P, S and Cl.

Halides and oxohalides: PCl$_3$, PCl$_5$, SOCl$_2$ and SO$_2$Cl$_2$

**(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 CO$_2$.

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

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

**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**


**Chemical Kinetics**


Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions. Comparison of the two theories (qualitative treatment only).
Reference Books:

- J. D. Lee: A New Concise Inorganic Chemistry, E.L.B.S.

CHEMISTRY LAB-DSC 2D LAB: CHEMISTRY OF S- AND P-BLOCK ELEMENTS, STATES OF MATTER & CHEMICAL KINETICS

60 Lectures

Section A: Inorganic Chemistry

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

Cations: NH$_4^+$, Pb$^{2+}$, Ag$^+$, Bi$^{3+}$, Cu$^{2+}$, Cd$^{2+}$, Sn$^{2+}$, Fe$^{3+}$, Al$^{3+}$, Co$^{2+}$, Cr$^{3+}$, Ni$^{2+}$, Mn$^{2+}$, Zn$^{2+}$, Ba$^{2+}$, Sr$^{2+}$, Ca$^{2+}$, K$^+$

Anions: CO$_3^{2-}$, S$^{2-}$, SO$_3^{2-}$, S$_2$O$_3^{2-}$, NO$_3^-$, CH$_3$COO$^-$, Cl$^-$, Br$^-$, I$^-$, NO$_3^-$, SO$_4^{2-}$, PO$_4^{3-}$, BO$_3^{3-}$, C$_2$O$_4^{2-}$, 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 H$_2$SO$_4$ by studying kinetics of hydrolysis of methyl acetate

Reference Books:
- A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

Discipline Specific Elective
Select two papers

CHEMISTRY-DSE I-IV (ELECTIVES)

CHEMISTRY-DSE: APPLICATIONS OF COMPUTERS IN CHEMISTRY
(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

Basics:
Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

Numerical methods:


Differential calculus: Numerical differentiation.

Integral calculus: Numerical integration (Trapezoidal and Simpson’s rule), probability distributions and mean values.

**Interpolation, extrapolation and curve fitting:** Handling of experimental data.

**Conceptual background of molecular modelling:** Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

**Reference Books:**

**PRACTICAL-DSE LAB: APPLICATIONS OF COMPUTERS IN CHEMISTRY**

**60 Lectures**

Computer programs based on numerical methods for
1. Roots of equations: (e.g. volume of van der Waals gas 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), probability distributions (gas kinetic theory) and mean values.

5. Simple exercises using molecular visualization software.

**Reference Books:**

**CHEMISTRY-DSE: ANALYTICAL METHODS IN CHEMISTRY**

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

Qualitative and quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals. (5 Lectures)

Optical methods of analysis:


UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;


Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

Structural illustration through interpretation of data, Effect and importance of isotope substitution.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples. (25 Lectures)

Thermal methods of analysis:

Theory of thermogravimetry (TG), basic principle of instrumentation.

Techniques for quantitative estimation of Ca and Mg from their mixture. (5 Lectures)

Electroanalytical methods:

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of $pK_a$ values. (10 Lectures)

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

Mechanism of extraction: extraction by solvation and chelation.

Technique of extraction: batch, continuous and counter current extractions.

Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.

Chromatography: Classification, principle and efficiency of the technique.

Mechanism of separation: adsorption, partition & ion exchange.

Development of chromatograms: frontal, elution and displacement methods.

Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Stereoisomeric separation and analysis: Measurement of optical rotation, calculation of Enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of enantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiral chromatographic techniques using chiral columns (GC and HPLC).

Role of computers in instrumental methods of analysis.

(15 Lectures)

Reference Books:

- Ditts, R.V. Analytical Chemistry – Methods of separation.

PRACTICALS- DSE LAB: ANALYTICAL METHODS IN CHEMISTRY
60 Lectures
I. Separation Techniques

1. Chromatography:

(a) Separation of mixtures

(i) Paper chromatographic separation of Fe$^{3+}$, Al$^{3+}$, and Cr$^{3+}$.

(ii) Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the $R_f$ values.

(b) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their $R_f$ values.

(c) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

II. Solvent Extractions:

(i) To separate a mixture of Ni$^{2+}$ & Fe$^{2+}$ by complexation with DMG and extracting the Ni$^{2+}$- DMG complex in chloroform, and determine its concentration by spectrophotometry.

(ii) Solvent extraction of zirconium with amberliti LA-1, separation from a mixture of irons and gallium.

3. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.

4. Determination of Na, Ca, Li in cola drinks and fruit juices using flame photometric techniques.

5. Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

(iii) Estimation of calcium, magnesium, phosphate, nitrate

6. Ion exchange:

(i) Determination of exchange capacity of cation exchange resins and anion exchange resins.

(ii) Separation of metal ions from their binary mixture.

(iii) Separation of amino acids from organic acids by ion exchange chromatography.

III Spectrophotometry
1. Determination of $pK_a$ values of indicator using spectrophotometry.

2. Structural characterization of compounds by infrared spectroscopy.

3. Determination of dissolved oxygen in water.

4. Determination of chemical oxygen demand (COD).

5. Determination of Biological oxygen demand (BOD).

6. Determine the composition of the Ferric-salicylate/ ferric-thiocyanate complex by Job’s method.

**Reference Books:**

- Ditts, R.V. Analytical Chemistry – Methods of separation.

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**CHEMISTRY-DSE: MOLECULAR MODELLING & DRUG DESIGN**  
(Credits: Theory-04, Practicals-02)

**Theory: 60 Lectures**

**Introduction to Molecular Modelling:**


(10 Lectures)

**Force Fields:**


(14 Lectures)

**Energy Minimization and Computer Simulation:**

(12 Lectures)

Molecular Dynamics & Monte Carlo Simulation:


(12 Lectures)

Structure Prediction and Drug Design:


Drug Discovery – Chemoinformatics – QSAR.

(12 Lectures)

Reference Books:

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PRACTICAL- DSE LAB: MOLECULA MODELLING & DRUG DESIGN

60 Lectures

i. 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.

ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of cis and trans 2-butene.

iii. 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.

iv. (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.

v. (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).

vi. 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.

vii. (a) 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.

viii. 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.

ix. (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:

CHEMISTRY-DSE: NOVEL INORGANIC SOLIDS
(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

Synthesis and modification of inorganic solids:


(10 Lectures)

Inorganic solids of technological importance:

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments.

Molecular material and fullerides, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

(10 Lectures)

Nanomaterials:
Overview of nanostructures and nanomaterials: classification.


(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:**


(10 Lectures)

**Reference Books:**

- Frank J. Ovens, Introduction to Nanotechnology

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CHEMISTRY PRACTICAL - DSE LAB: NOVEL INORGANIC SOLIDS
60 Lectures
1. Determination of cation exchange method
2. Determination of total difference of solids.
3. Synthesis of hydrogel by co-precipitation method.

Reference Book:

CHEMISTRY-DSE: 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:

(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** \((M_n, M_w, \text{etc})\) 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:**
- *Seymour’s Polymer Chemistry*, Marcel Dekker, Inc.

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**CHEMISTRY PRACTICAL - DSE LAB: POLYMER CHEMISTRY**

**60 Lectures**

1. 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-isobutylonitrile (AIBN)
2. Preparation of nylon 66/6
   1. 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).
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:
- Malcom P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
• Seymour/ Carraher’s Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

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CHEMISTRY-DSE: RESEARCH METHODOLOGY FOR CHEMISTRY (Credits: Theory-05, Tutorials-01)
Theory: 75 Lectures

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.


(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, style, 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.


(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**

- OSU safety manual 1.01.

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**CHEMISTRY-DSE: GREEN CHEMISTRY**

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

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, solventless 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 Strecke synthesis), citral, ibuprofen, paracetamol, furfural.
2. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzole 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, Cannizaro reaction, Streaker synthesis, Reformatsky reaction.
4. Selective methylation of active methylene group using dimethylcarbonate: Solid-state polymerization of amorphous polymers using diphenylcarbonate; Use of “Clayan”, 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 solventless reactions; oncovalent derivatization; Green chemistry in sustainable development. (8 Lectures)

Reference Books:

CHEMISTRY PRACTICAL - DSE 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.

- Effect of concentration on clock reaction
- 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 stimulate 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$^-\rightarrow$ propene + trimethylpropene + water
(II) $\text{C}_3\text{H}_7\text{OH} \xrightarrow{\text{H}_2\text{SO}_4/\Delta} \text{propene} + \text{water}$

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.


7. Mechanochemical solvent free synthesis of azomethines

8. Co-crystal controlled solid state synthesis ($\text{C}_2\text{S}_3$) 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. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

**Reference Books:**

- Pavia, D. L. Lamponan, G. H. & Kriz, G.S. *W B Introduction to organic laboratory*

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**CHEMISTRY-DSE: INDUSTRIAL CHEMICALS AND ENVIRONMENT**

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

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


Pollution by SO₂, CO₂, CO, NOₓ, H₂S and other foul smelling gases. Methods of estimation of CO, NOₓ, SOₓ 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:


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**CHEMISTRY PRACTICAL - DSE 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 (AgNO₃ and potassium chromate).
6. Estimation of total alkalinity of water samples (CO₃²⁻, HCO₃⁻) using double titration method.
8. Study of some of the common bio-indicators of pollution.
10. Preparation of borax/ boric acid.

Reference Books:


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CHEMISTRY-DSE: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE
(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

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: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

(16 Lectures)

Fertilizers:

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

(8 Lectures)

Surface Coatings:


(10 Lectures)
**Batteries:**

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.

*(6 Lectures)*

**Alloys:**

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

*(10 Lectures)*

**Catalysis:**

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

Phase transfer 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.

*(4 Lectures)*

**Reference Books:**

PRACTICALS-DSE LAB: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

60 Lectures
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.
8. Preparation of pigment (zinc oxide).

Reference Books:
- B. K. Sharma: Engineering Chemistry, Goel Publishing House, Meerut

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

Theory: 60 Lectures

Introduction to spectroscopic methods of analysis:
Recap of the spectroscopic methods covered in detail in the core chemistry syllabus:
Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiation.

(4 Lectures)

Molecular spectroscopy:

Infrared spectroscopy:
Interactions with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution),
advantages of Fourier Transform (FTIR). Samples and results expected. Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.

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

(16 Lectures)

**Separation techniques**

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

**Immunoassays and DNA techniques**

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

(16 Lectures)

**Elemental analysis:**

Mass spectrometry (electrical discharges).


Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

(8 Lectures)

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

(4 Lectures)
Electroanalytical Methods: Potentiometry & Voltammetry

Radiochemical Methods

X-ray analysis and electron spectroscopy (surface analysis)

Reference books:
- Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.
- P.W. Atkins: Physical Chemistry.
- G.W. Castellan: Physical Chemistry.
- C.N. Banwell: Fundamentals of Molecular Spectroscopy.
- W.J. Moore: Physical Chemistry.

PRACTICALS-DSE LAB: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS
60 Lectures

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

*At least 10 experiments to be performed.*

**Reference Books:**
- Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.

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**DSE: CHEMISTRY OF D-BLOCK ELEMENTS, QUANTUM CHEMISTRY & SPECTROSCOPY**

*(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.

Lanthanoids and actinoids: Electronic configurations, oxidation states, colour, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only).

*(12 Lectures)*

**Coordination Chemistry**


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 $O_h$ and $T_d$ complexes, Tetragonal distortion of octahedral geometry.
Jahn-Teller distortion, Square planar coordination.  

(10 Lectures)

Section B: Physical Chemistry-4 (30 Lectures)

Quantum Chemistry & Spectroscopy


Postulates of quantum mechanics, quantum mechanical operators.

Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wavefunctions, 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.


(24 Lectures)

Photochemistry


(6 Lectures)

Reference Books:
DSE LAB
60 Lectures

Section A: Inorganic Chemistry

1. Estimation of the amount of nickel present in a given solution as bis(dimethylglyoximato) nickel(II) or aluminium as oxinate in a given solution gravimetrically.
2. Estimation of (i) Mg$^{2+}$ or (ii) Zn$^{2+}$ by complexometric titrations using EDTA.
3. Estimation of total hardness of a given sample of water by complexometric titration.
4. To draw calibration curve (absorbance at $\lambda_{max}$ vs. concentration) for various concentrations of a given coloured compound and estimate the concentration of the same in a given solution.
5. 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

I. Study the 200-500 nm absorbance spectra of KMnO$_4$ and K$_2$Cr$_2$O$_7$ (in 0.1 M H$_2$SO$_4$) and determine the $\lambda_{max}$ values. Calculate the energies of the two transitions in different units (J molecule$^{-1}$, kJ mol$^{-1}$, cm$^{-1}$, eV).
II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of K$_2$Cr$_2$O$_7$.
III. 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.

Colourimetry

I. Verify Lambert-Beer’s law and determine the concentration of CuSO$_4$/KMnO$_4$/K$_2$Cr$_2$O$_7$ in a solution of unknown concentration
II. Analyse the given vibration-rotation spectrum of HCl(g)

Reference Books:
- A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
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, K₂Cr₂O₇, KMnO₄, K₄[Fe(CN)₆], sodium nitroprusside, [Co(NH₃)₆]Cl₃, Na₃[Co(NO₂)₆].

(6 Lectures)

Organometallic Compounds

Definition and Classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeiss 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 Mg²⁺ ions: Na/K pump; Role of Mg²⁺ ions in energy production and chlorophyll. Role of Ca²⁺ in blood clotting, stabilization of protein structures and structural role (bones).

(12 Lectures)

Section B: Organic Chemistry-4 (30 Lectures)

Polynuclear and heteronuclear aromatic compounds:
Properties of the following compounds with reference to electrophilic and nucleophilic substitution: Naphthalene, Anthracene, Furan, Pyrrole, Thiophene, and Pyridine.

(6 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, $\lambda_{\text{max}}$ & $\varepsilon_{\text{max}}$, chromophore, auxochrome, bathochromic and hypsochromic shifts. Application of electronic spectroscopy and Woodward rules for calculating $\lambda_{\text{max}}$ of conjugated dienes and $\alpha,\beta$-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).

(18 Lectures)

Reference Books:

- J.D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.

DSE LAB

60 Lectures

Section A: Inorganic Chemistry
1. Separation of mixtures by chromatography: Measure the $R_f$ value in each case. (Combination of two ions to be given)

Paper chromatographic separation of Fe$^{3+}$, Al$^{3+}$ and Cr$^{3+}$ or

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

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

Reference Books:

DSE: MOLECULES OF LIFE

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Carbohydrates (10 Periods)

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 monosacharides, structure of disaccharides (sucrose, maltose, lactose) and polysacharides (starch and cellulose) excluding their structure elucidation.

Unit 2: Amino Acids, Peptides and Proteins (12 Periods)
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 (t-butyloxycarbonyl and pthaloyl) & C-activating groups and Merrifield solid phase synthesis.

Unit 3: Enzymes and correlation with drug action (12 Periods)

Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, Specificity of enzyme action (Including stereospecificity), Enzyme inhibitors and their importance, phenomenon of inhibition (Competitive and Non competitive inhibition including allosteric inhibition). Drug action-receptor theory. Structure –activity relationships of drug molecules, binding role of –OH group, -NH$_2$ group, double bond and aromatic ring.

Unit 4: Nucleic Acids (10 Periods)

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 Periods)

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 Periods)


Recommended Texts:
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
• Finar, I. L. *Organic Chemistry (Volume 2)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

**DSE LAB**

**60 Lectures**
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 synthesise aspirin by acetylation of salicylic acid and compare it with the ingredient of an aspirin tablet by TLC.

**Recommended Texts:**
Skill Enhancement Course (any four) (Credit: 02 each)- SEC1 to SEC4

Chemistry
IT SKILLS FOR CHEMISTS
(Credits: 02)
30 Lectures

Mathematics

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

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


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

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

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

Computer programming:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

BASIC programs for curve fitting, numerical differentiation and integration (Trapezoidal rule, Simpson’s rule), finding roots (quadratic formula, iterative, Newton-Raphson method).
HANDS ON

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

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

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

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

**Presentation:** Presentation graphics

**Reference Books:**

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**BASIC ANALYTICAL CHEMISTRY**

(Credits: 02)

30 Lectures
Introduction: Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation of experimental data and results, from the point of view of significant figures.

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

a. Determination of pH of soil samples.
b. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

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

a. Determination of pH, acidity and alkalinity of a water sample.
b. Determination of dissolved oxygen (DO) of a water sample.

Analysis of food products: Nutritional value of foods, idea about food processing and food preservations and adulteration.

a. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
b. Analysis of preservatives and colouring matter.

Chromatography: Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.

a. Paper chromatographic separation of mixture of metal ion (Fe$^{3+}$ and Al$^{3+}$).
b. To compare paint samples by TLC method.

Ion-exchange: Column, ion-exchange chromatography etc. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Analysis of cosmetics: Major and minor constituents and their function

a. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
b. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Suggested Applications (Any one):

a. To study the use of phenolphthalein in trap cases.
b. To analyze arson accelerants.
c. To carry out analysis of gasoline.

Suggested Instrumental demonstrations:

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

Reference Books:

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CHEMICAL TECHNOLOGY & SOCIETY
(Credits: 02)
Theory: 30 Lectures

Chemical Technology

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

Society

Exploration of societal and technological issues from a chemical perspective. Chemical and scientific literacy as a means to better understand topics like air and water (and the trace materials found in them that are referred to as pollutants); energy from natural sources (i.e. solar and renewable forms), from fossil fuels and from nuclear fission; materials like plastics and polymers and their natural analogues, proteins and nucleic acids, and molecular reactivity and interconversions from simple examples like combustion to complex instances like genetic engineering and the manufacture of drugs.

Reference Book:
CHEMoinformatics
(Credits: 02)
Theory: 30 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; Modeling 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:

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.

**Reference**

[www.rsc.org](http://www.rsc.org)

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**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


Reference Books:
MANJULA GURU & M.B. RAO, UNDERSTANDING TRIPS: MANAGING KNOWLEDGE IN DEVELOPING COUNTRIES, SAGE PUBLICATIONS (2003).


JAYASHREE WATAL, INTELLECTUAL PROPERTY RIGHTS IN THE WTO AND DEVELOPING COUNTRIES, OXFORD UNIVERSITY PRESS, OXFORD.

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ANALYTICAL CLINICAL BIOCHEMISTRY
(CREDITS: 02)

THEORY: 30 LECTURES

Basic understanding of the structures, properties and functions of carbohydrates, lipids and proteins:

Review of concepts studied in the core course:

Carbohydrates: Biological importance of carbohydrates, Metabolism, Cellular currency of energy (ATP), Glycolysis, Alcoholic and Lactic acid fermentations, Krebs cycle.

Isolation and characterization of polysaccharides.

Proteins: Classification, biological importance; Primary and secondary and tertiary structures of proteins: α-helix and β-pleated sheets, Isolation, characterization, denaturation of proteins.

Enzymes: Nomenclature, Characteristics (mention of Ribozymes), Classification; Active site, Mechanism of enzyme action, Stereospecificity of enzymes, Coenzymes and cofactors, Enzyme inhibitors, Introduction to Biocatalysis: Importance in “Green Chemistry” and Chemical Industry.

Lipids: Classification. Biological importance of triglycerides and phosphoglycerides and cholesterol; Lipid membrane, Liposomes and their biological functions and underlying applications.

Lipoproteins.

Properties, functions and biochemical functions of steroid hormones.

Biochemistry of peptide hormones.

Structure of DNA (Watson-Crick model) and RNA, Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation, Introduction to Gene therapy.

Enzymes: Nomenclature, classification, effect of pH, temperature on enzyme activity, enzyme inhibition.
Biochemistry of disease: A diagnostic approach by blood/ urine analysis.

**Blood:** Composition and functions of blood, blood coagulation. Blood collection and preservation of samples. Anaemia, Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

**Urine:** Collection and preservation of samples. 6. Formation of urine. Composition and estimation of constituents of normal and pathological urine.

**Practicals**

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.
7. Isolation of protein.
8. Determination of protein by the Biuret reaction.
9. Determination of nucleic acids

**Reference Books:**
- T.G. Cooper: Tool of Biochemistry.
- Alan H Gowenlock: Varley’s Practical Clinical Biochemistry.

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**GREEN METHODS IN CHEMISTRY**

(Credits: 02)

**Theory:** 30 Lectures

Tools of Green chemistry, Twelve principles of Green Chemistry, with examples.

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

1. A green synthesis of ibuprofen which creates less waste and fewer byproducts (Atom economy).
2. Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO$_2$ for precision cleaning and dry cleaning of garments.
3. Environmentally safe antifoulant.
4. CO$_2$ as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market.
5 Using a catalyst to improve the delignifying (bleaching) activity of hydrogen peroxide.
6 A new generation of environmentally advanced preservative: getting the chromium and arsenic out of pressure treated wood.
7 Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
8 Development of a fully recyclable carpet: cradle to cradle carpeting.

Reference Books:


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PHARMACEUTICAL CHEMISTRY
(Credits: 02)

Theory: 30 Lectures

Drugs & Pharmaceuticals
Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, Ibuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

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

Practicals
1. Preparation of Aspirin and its analysis.
2. Preparation of magnesium bisilicate (Antacid).

Reference Books:


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CHEMISTRY OF COSMETICS & PERFUMES
(Credits: 02)
30 Lectures

A general study including preparation and uses of the following: Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

Practicals
1. Preparation of talcum powder.
2. Preparation of shampoo.
3. Preparation of enamels.
4. Preparation of hair remover.
5. Preparation of face cream.
6. Preparation of nail polish and nail polish remover.

Reference Books:

Pesticide Chemistry
(Credits: 02)

30 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
2  To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
3  Preparation of simple organophosphates, phosphonates and thiophosphates

Reference Book:

Fuel Chemistry
(Credits: 02)
30 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:

--------------------------------------------------------------------------------------------------
Note:

1. In all 72 credits are to be completed in M.Sc. out of which 18 credits shall be taken by the student in one semester.
2. In semester III and IV the student will opt one branch out of three branches i.e. Inorganic, Organic and Physical according to the availability of faculty in the department. The student will also take 18 credits in III and IV semesters out of which 9 credits i.e. two core courses will be compulsory and rest of 9 credits will be from elective courses.

M.S.c. I

Semester I

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M.S.c. III

Semester III

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<td>Spectroscopy &amp; Solid State</td>
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<td>Organometallic reagents and</td>
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### [C] Physical Chemistry
1. Laboratory Course Physical IIIA C019 100 3
2. Laboratory Course Physical IIIB C020 100 3
3. Chemistry of Materials C021 100 3
4. Spectroscopy, X-ray & Solid State E001 100 3
5. Bioinorganic, Bioorganic and Biophysical Chemistry I E002 100 3
6. Analytical Chemistry E004 100 3
7. Liquid State E008 100 3

### M.Sc. II
#### Semester IV

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### Self Study Courses

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Unit I
Stereochemistry and Bonding in Main Group Compounds
VSEPR, Walsh diagrams (tri-atomic molecules), dπ-pπ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Unit II
Metal- Ligand Equilibria in Solution
Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectroscopy.

Unit III
Reaction Mechanism of Transition Metal Complexes
Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer and inner sphere type reactions.

Unit IV
Metal- Ligand Bonding
Limitations of crystal field theory. Jahn-Teller distortion. Evidence of covalent character in Metal-Ligand bonding. Molecular orbital theory as applied to octahedral, tetrahedral and square planar complexes.

Books suggested
Unit I
Nature of Bonding in Organic Molecules
Hyperconjugation, bonding in fullerenes, tautomerism.
Aromaticity in benzenoid and non benzenoid compounds, alternant and non alternant hydrocarbons.
Huckel’s rule, energy level of π-molecular orbitals, annulenes, antiaromaticity, homo-aromaticity, PMO approach.
Bonds weaker than covalent, crown ether complexes and cryptands, inclusion compounds, cyclodextrin, catenanes and rotaxanes.

Unit II
Stereochemistry
Conformational analysis of cycloalkane, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis, chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit III
Reaction Mechanism : Structure and Reactivity
Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond’s postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Effect of structure on reactivity – resonance and field effects, steric effect, quantitative treatments. Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

Unit IV
Aliphatic Nucleophilic Substitution
$S_N1$, $S_N2$ and mixed $S_N1$ and $S_N2$ mechanism. The neighbouring group mechanism, neighbouring group participation (by π- and σ bonds). Anchimeric assistance. $S_N1$ mechanism- Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophilic group, leaving group and reaction medium, ambident nucleophile.

Unit V
Aliphatic Electrophilic Substitution
Bimolecular mechanism- SE2 and SEi. The SE1 mechanism, electrophilic substitution accompanied by double bond shift. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Books suggested
Unit I
Quantum Chemistry

A. Introduction to Exact Quantum Mechanical Results
The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

B. Approximate Methods
The variation theorem, linear variation principle, perturbation theory (first order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

C. Angular Momentum
Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

D. Electronic Structure of Atoms
Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the \( p^\pi \) configuration, term separation energies for the \( d^\pi \) configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.

Thermodynamics

A. Classical Thermodynamics
Unit II
Surface Chemistry
A. Adsorption
Surface tension, capillary actions, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon), catalytic activity at surfaces.

B. Micelles
Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

C. Macromolecules
Polymer-definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and, light scattering methods sedimentation), chain configuration of macromolecules, calculation of average dimensions of various chain structures.

Books suggested
1. Physical Chemistry, P.W. Atkins, ELBS.
4. Coulson’s Valence, R. McWeeny, ELBS.

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Unit I
Symmetry and Group Theory in Chemistry
Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroups, conjugacy relation and classes. Point symmetry group, Schonflies symbols, representations of groups by matrices (representation for the Cn, Cnv, Cnh, Dnh etc. group to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use in spectroscopy.

Unit II
Unifying Principles
Electromagnetic radiation, interaction of electromagnetic radiation with matter. Absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Uncertainty relation and
natural line width and natural line broadening, transition probability, result of the time dependent perturbation theory, transition moment, selection rules, intensity of special lines, Born-oppenheimer approximation, rotational, and electronic energy levels.

Unit III
Atomic Electronic Spectroscopy
Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

Unit IV
Microwave Spectroscopy
Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, Stark effect, nuclear and electron spin interaction and effect of external field. Applications.

Unit V
Infrared Spectroscopy
Review of linear harmonic oscillator, vibrational energies of diatomic molecules, Zero point energy, force constant and bond strengths; anharmonicity. Morse potential energy diagram, vibration-rotation spectroscopy; P,Q,R branches. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region., metal-ligand vibrations.

Books Suggested

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Note: The duration of examination will be of eight hours. Students are required to do one practical of 20 marks each from Inorganic, Organic and Physical sections. Each exercise will be 20 marks. Viva 15 marks Seminar/Attendance/Assessment/Record 25 marks.

Inorganic Chemistry

Qualitative Analysis
Qualitative analysis of mixture by semi-micro method containing not more than six cations and anions including:
(i). Rare-earth elements
(ii). Anions, which have not been done in under graduate practical.
(iii). Insolubles.
Organic Chemistry

Qualitative Analysis
Separation, purification and identification of compounds of binary mixture (solid-solid or liquid and solid) using TLC and Paper Chromatography, chemical tests and spectroscopic analysis.

Physical Chemistry

Chemical Kinetics
1. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
2. Determination of the velocity constant of hydrolysis of an ester.
3. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics of the reaction.
4. Flowing clock reactions (Ref: Experiments in Physical Chemistry by Showmaker).
5. Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).

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Note: The duration of examination will be of eight hours. Students are required to do one practical each from Inorganic, Organic and Physical sections. Each exercise will be 20 marks.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

Inorganic Chemistry

Chromatography
Separation of cations and anions by-
Paper Chromatography
Thin Layer Chromatography
Ion Exchange Chromatography

Organic Chemistry

Organic Synthesis
Acetylation: Acetylation
Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.
Grignard reaction: Synthesis of triphenylmethanol from benzoic acid.
Sandmeyer reaction: p-Chlorotoluene from p-toluene
Physical Chemistry

Electrochemistry
Conductometry
1. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
2. Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO₄, BaSO₄) conductometrically.
3. Determination of the strength of strong and weak acids in a given mixture conductometrically.
4. To study the effect of solvent on the conductance of AgNO₃/CH₃COOH and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
5. Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel’s limiting law.

Semester- II

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<th>Inorganic Chemistry - II</th>
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Unit I
Electronic Spectra & Magnetic Properties of Transaction Metal Complexes

Unit II
Metal-π-Complexes
Important reactions, preparation, bonding and structure of metal carbonyls, metal nitrosyls and dinitrogen complexes. Vibrational spectra of metal carbonyls and nitrosyls for bonding and structure elucidation.
Tertiary phosphine as ligand.

Unit III
Metal Clusters

Unit IV
Silicates
Classification and structure. Asbestos and zeolites. Silicates in technology.

Books suggested

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<th>SOS/C008</th>
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Unit I
Aromatic Electrophilic Substitution
Orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrate and electrophiles. Diazonium coupling, Vilsmeir Haak reaction, Gattermann-Koch reaction.

Unit II
Aromatic Nucleophilic Substitution
The SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity- effect of substrate structure, leaving group and attacking nucleophile. The von Rictor, Sommelet-Hauser, and Smiles rearrangements.

Unit III
Free Radical Reactions

Unit IV
Addition to Carbon-Carbon Multiple Bonds

Unit V
Addition to Carbon-Hetero Multiple Bonds
Unit VI
Elimination Reactions
The E2, E1 and E1cB mechanisms and their stereochemistry. Orientation of the double bond. Reactivity- effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Unit VII
Pericyclic Reactions

Books suggested

Unit I
Chemical Dynamics
Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction), homogeneous catalysis, kinetics of enzymes reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.
Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

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<th>Physical Chemistry II</th>
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Unit II
Statistical Thermodynamics
Heat capacity behaviour of solids- chemical equilibria and chemical equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics – distribution law and application to helium.

Non-Equilibrium Thermodynamics
Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager’s reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

Unit III
Electrochemistry


Books suggested
1. Physical Chemistry, P.W. Atkins, ELBS.
2. Coulson’s Valence, R. McWeeny, ELBS.

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<th>SOS/C010</th>
<th>Spectroscopy and Separation Methods</th>
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Unit I
Molecular Electronic Spectroscopy
Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra, radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge transfer spectra.
Unit II
**Raman Spectroscopy**

Unit III
**Magnetic Resonance Spectroscopy**

**Nuclear Magnetic Resonance Spectroscopy**
Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factor influencing chemical shift, deshielding, spin-spin interaction, factors influencing coupling constant ‘J’. Classification (ABX, AMX, ABC, A₂B₂ etc.), spin decoupling, basic ideas about instrument, NMR studies of nuclei other than proton-¹³C, ¹⁹F and ³¹P. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

Unit IV
**Chromatographic Methods**
Principle, instrumentation and applications of gas liquid chromatography and HPLC. Ion exchange chromatography: cationic and anionic exchanges and their applications. Van-Deemter equation (no derivation), concept about HEPT-plate theory and rate theory. Applications.

Unit V
**Radio Analytical Methods**
Basic principles and types of measuring instruments, isotope dilution techniques: principle of operations and uses. Applications.

**Books Suggested**
2. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.

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Note: The duration of examination will be of eight hours. Students are required to do one practical each from Inorganic, Organic and Physical sections. Each exercise will be 20 marks.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.
Inorganic Chemistry

Quantitative Analysis
Quantitative Analysis of mixtures of two metal ions involving Volumetric (by complexometric titration using masking and demasking agents) and gravimetric analysis.

Organic Chemistry

Organic Synthesis
Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetocetate by A.E.E. condensation.
Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate
Aromatic electrophilic Substitutions: Synthesis of p-nitroaniline and p-bromoaniline.
The products may be characterized by Spectral Techniques where possible.

Physical Chemistry

Solutions
1. Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
2. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

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Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

Inorganic Chemistry

Preparations
Preparation of selected inorganic compounds:
VO (acac)_2
TiO (C_9H_8NO)_2. 2H_2O
cis-K[Cr(C_2O_4)_2 (H_2O)_2]
Na[Cr(NH_3)_2(SCN)_4]
Mn (acac)_3
K_3 [Fe (C_2O_4)_3] 3H_2O
Prussian Blue, Tumbull’s Blue
Co [(NH_3)_6] Cl_3
[Cu (en)_2 (H_2O)_2] I_2
Cu_2HgI_4
Organic Chemistry

Quantitative Analysis
Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
Estimation of amines/phenols using bromate bromide solution/or acetylation method.
Determination of Iodine and Saponification values of an oil sample
Determination of DO, COD and BOD of water sample.

Physical Chemistry

Electrochemistry

Potentiometry/pH-metry
1. Determination of strengths of halides in a mixture potentiometrically.
2. Determination of the valency of mercurous ions potentiometrically.
3. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
5. Determination of the formation constant of silver-ammonia complex and stiochiometry of the complex potentiometrically.
6. Acid-base titration in a non-aqueous media using a pH meter.
8. Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
10. Determination of thermodynamic constants $\Delta G$, $\Delta S$ and $\Delta H$ for the reaction by e.m.f. method.

$$\text{Zn} + \text{H}_2\text{SO}_4 \rightarrow \text{ZnSO}_4 + 2\text{H}$$

Semester- III

Inorganic Chemistry

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Note: The duration of examination will be of eight hours. Students are required to do one practical of 60 marks.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.
Synthesis of selected inorganic compounds/complexes and their characterization by IR, electronic spectra (UV & Visible), NMR, Mossbauer, ESR and magnetic susceptibility etc. measurement. Selection can be made from the following or any other from the existing literature.

(i). Cis and Trans isomers of \([\text{Co(en)}_2\text{Cl}_2]\) Cl.

(ii). Metal acetylacetonates: \(\text{Cr(acac)}_3\); Vanadyl acetylacetonate, \(\text{Cu(acac)}_2\) H\(_2\)O etc.

(iii). Ferrocene

(iv). \(\text{Cr(III)}\) complexes: \([\text{Cr(H}_2\text{O)}_6]\)(NO\(_3\))\(_3\)3H\(_2\)O;\([\text{Cr(H}_2\text{O)}_4\text{Cl}_2]\) Cl.2H\(_2\)O; \([\text{Cr(en)}_3]\)Cl\(_3\)

(v). Tin (IV) iodide, Tin (IV) chloride, Tin (II) iodide.


(viii). Reaction of \(\text{Cr (III)}\) with multidentate ligand, a kinetic experiment (visible spectra of \(\text{Cr-EDTA complex})\).

(ix). Other new synthesis reported in literature.

(x). Bromination of \(\text{Cr (acac)}_3\).

(xi). Preparation of copper glycine complex-cis and trans bis glycinato copper (II).

(xii). Relative stability of Tin (IV) and Pb (IV), Preparation of ammonium hexachlorostannate,\((\text{NH}_4)_2\text{SnCl}_6\) and ammonium hexachloroplumbate; \((\text{NH}_4)_2\text{PbCl}_6\).

Books Suggested
1. Vogel’s Text Book of Qualitative Analysis, ELBS .
2. Vogel’s Text Book of Quantitative Analysis, ELBS.

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Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

Analysis of ores, alloys and inorganic substances by various chemical methods.

Books Suggested
4. Vogel’s Text Book of Qualitative Analysis, ELBS .
5. Vogel’s Text Book of Quantitative Analysis, ELBS.
I. Alkyls and Aryls of Transition Metals

II. Compounds of Transition metal-carbon multiple bonds
Alkylidenes, alkyldynes, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

III. Transition Metal π-Complexes
Transition Metal π-Complexes with unsaturated organic molecules. Alkenes, alkynes, allyl, diene, dienyl, arene and trieny compounds; preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

IV. Metal Compounds with bonds to Hydrogen
Transition metal compounds with bonds to hydrogen.

V. Homogeneous Catalysis
Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reaction, activation of C-H bond.

VI. Fluxional Organometallic Compounds
Fluxionality and dynamic equilibria in compounds such as \(\eta^2\)-olefin, \(\eta^3\)-allyl and dienyl complexes, their characterization.

Books Suggested
5. Organometallic Compounds, NLH Green, Chapman & Hall, U.K.
I. **Ultraviolet and Visible Spectroscopy**
Instrumentation, source, monochromators, detectors, single and double beam instruments, applications.

II. **Infrared Spectroscopy**
Instrumentation, source, monochromators, optics of double beam instruments, detectors, sample preparation, applications.

III. **X-Ray Diffraction**

IV. **Electron Diffraction**
Scattering intensity vs. scattering angle, Wire equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

V. **Neutron Diffraction**
Scattering of neutrons by solids and liquids, magnetic scattering, measuring techniques. Elucidation of structure of magnetically ordered unit cell.

VI. **Solid State Chemistry**

**Solid State Reactions**
General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

**Books Suggested:**

A) Bioinorganic Chemistry

I. Metal Ions in Biological Systems, Na⁺/K⁺ Pump

II. Bioenergetics and ATP Cycles
DNA polymerization, glucose storage, metal complexes in transmission of energy; chlorophylls, photo system I and photo system II in cleavage of water. Model systems.

III. Transport and Storage of Dioxygen
Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

B) Bioorganic Chemistry

I. Enzymes & Mechanism of Enzyme Action
Introduction and historical perspective, chemical and biological catalysis, properties of enzymes-catalytic power, specificity and regulation. Fischer’s lock and Koshland’s induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed, mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition. Transition-state theory, acid-base catalysis, covalent catalysis, strain of distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

II. Kinds of Reactions Catalysed by Enzymes
Nucleophillic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, β-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

C) Biophysical Chemistry

I. Biological Cell and its Constituents, Cell Membrane and Transport of Ions
Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition. Structure and functions of cell membrane, ion transport through cell membrane.

II. Bioenergetics
Standard free energy change in biological reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

Books Suggested
Unit I
**Metal Storage Transport and Biominalization**
Ferritin, Transferrin, and siderophores

Unit II
**Calcium in Biology**
Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins.

Unit III
**Metalloenzymes**

Unit IV
**Metal-Nucleic Acid Interactions**
Metal ions and metal complex interactions. Metal complexes-nucleic acids.

Unit V
**Metals in Medicine**
Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

Unit VI
**Supramolecular Chemistry**
Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co-receptor molecules and multiple recognition. H-bonds in supramolecular structures. Use of H-bond in crystal engineering and molecular recognition. Chelate and

Books Suggested
1. Supramolecular Chemistry, J.M. Lehn, VCH.

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<th>SOS/E004</th>
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Unit I
Introduction

Unit II
Errors
Determinate and indeterminate errors, minimization of determinate errors, random distribution of indeterminate errors.

Unit III
Statistical data analysis
Accuracy and precision, significant figures and computations, mean and standard deviation, distribution of random errors, reliability of results, confidence interval, comparison of results, comparison of means of two samples, paired t-test, number of replicate determinations and its use, correlation and regression, linear regression, analysis of variance, rejection of data.

Unit IV
Application of analytical chemistry in the study of water and soil pollutions, analysis of fuel, body fluids and drugs.

Books Suggested
Organic Chemistry

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Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

Qualitative Analysis
Separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and one solid, two solids and one liquid), using TLC for checking the purity of the separated compounds. Preparation of derivatives and spectral analysis.

Books Suggested

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Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

Multi-step Synthesis of Organic Compounds
The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

Photochemical reaction
Benzophenone → Benzpinacol → Benzpinacolone
Beckmann rearrangement: Benzanilide from benzene
Benzene → Benzophenone → Benzophenone oxime → Benzanilide
Benzilic acid rearrangement: Benzilic acid from benzoin
Benzoin → Benzil → Benzilic acid

**Synthesis of heterocyclic compounds**

**Enzymatic Synthesis**
Enzymatic reduction: Reduction of ethyl acetoacetate using Baker’s yeast to yield enantiomeric excess of S (+) ethyl-3-hydroxybutanoate and determine its optical purity.
Biosynthesis of ethanol from sucrose

**Synthesis using microwaves**
Alkylation of diethyl malonate with benzyl chloride.
Synthesis using phase transfer catalyst.
Alkylation of diethyl malonate or ethylacetoacetate with an alkyl halide.

**Books Suggested**

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<th>Organic Synthesis and Photochemistry</th>
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**Unit I**
**Disconnection Approach**
An introduction to synthons and synthetic equivalents disconnection approach, functional group interconversions, the importance of order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions and amine synthesis.

**Unit II**
**Protecting Groups**
Principle of protection of alcohols, amine, carbonyl and carboxyl groups

**Unit III**
**One Group and Two Group C-C Disconnections**
Alcohols and carbonyl compounds regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis. Diels-Alder reaction, 1,3-difunctional compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensations. Micheal addition and Robinson annelation.

**Unit IV**
Determination of Reaction Mechanism
Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions, photo-dissociation, gas-phase photolysis.

Unit V
Photochemical Reactions
Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.
Intramolecular reactions of carbonyl compounds-saturated cyclic and acyclic, β,γ-unsaturated and α,β-unsaturated compounds. Cyclohexadienones.
Intramolecular cycloaddition reactions-dimerisation and oxetane formation.
Isomerisation, additions and substitutions. Photo-Fries rearrangement, Barton reaction.

Books Suggested
10. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication
11. Molecular Photochemistry, N.J. Turro, W.A. Benjamin

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Unit I
Ultraviolet and Visible Spectroscopy
Effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds.

Unit II
Infrared Spectroscopy
General idea of the vibrational frequencies of aliphatic and aromatic hydrocarbons, amines, carbonyl compounds, acid and acid derivatives and conjugated carbonyl compounds, effect of hydrogen bonding and solvent on IR.

Unit III
Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)
Definition, deduction of absolute configuration and octant rule for ketones.

Unit IV
Solid State Chemistry
(a). Solid State Reactions
General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

(b). Organic Solids, Fullerene, Molecular devices
Electrically conducting solids, organic charge transfer complex, organic metals, magnetism in organic materials, fullerenes and doped fullerenes, organic superconductors, molecular rectifiers, transistors, artificial photosynthetic devices, molecular memory, switches and sensors.

Books Suggested

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<th>SOS/E006</th>
<th>Organometallic Reagents and Organic Synthesis</th>
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Unit I
Principles, preparations, properties and applications of the following in organic synthesis with mechanistic details.

Group I and II metal organic compounds
Li and Hg compounds.
Transition metals
Pd, Ni and Cr compounds.
Other elements
Si and B compounds.

Unit II
Oxidation
Introduction. Different oxidative processes.
Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and inactivated).
Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids.
Amines, hydrazines, and sulphides.
Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate.

Unit III
Reduction
Introduction. Different reductive processes.
Reduction of hydrocarbons- alkenes, alkynes and aromatic rings.
Reduction of carbonyl compounds (aldehydes, ketones, acids and their derivatives). Epoxides.
Reduction of nitro, nitroso, azo and oxime groups.
Hydrogenolysis.

Unit IV
Rearrangements
General mechanistic considerations-nature of migration, migratory aptitude, memory effects
A detailed study of the following rearrangements
Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction

Unit V
Metallocenes, Nonbenzenoid Aromatics and Polycyclic Aromatic Compounds
General considerations, synthesis and reactions of some representative compounds

Books Suggested

SOS/E007 Medicinal Chemistry
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Unit I
Drug Design

**Unit II**
**Pharmacokinetics**
Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

**Unit III**
**Pharmacodynamics**
Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotic, biotransformation, significance of drug metabolism in medicinal chemistry.

**Unit IV**
**Antineoplastic Agents**

**Unit V**
**Antibiotics**

**Books suggested**
1. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.

**Physical Chemistry**

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Note: The duration of examination will be of eight hours. Students are required to do one practical of 60 marks.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

1. Verification of the law of photochemical equivalence.
2. Order of reaction by:
   (a). Isolation Method.
   (b). Half life period method
   (c). Integration method
3. Temperature coefficient of a reaction.
4. Energy of activation of a reaction.
5. Entropy of a reaction.
6. Determination of pH by following methods:
   (a). Electrical Conductivity.
   (b). E.M.F.
   (c). Polarography

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Note: The duration of examination will be of eight hours. Students are required to do one practical of 60 marks.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

1. Hydrolysis of the salts by following methods:
   (a). Cryoscopic
   (b). Electrical Conductivity.
   (c). E.M.F.
2. Study of complex formation by the following methods and determination of stability constant wherever practicable:
   (a). Cryoscopic
   (b). Electrical Methods.
   (c). E.M.F.
3. Determination of solubility of sparingly soluble salts by the following methods:
   (a). Electrical Conductivity.
   (b). E.M.F.
4. Dissociation constants of polybasic acids.

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<th>Chemistry of Materials</th>
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Unit I
Multiphase Materials
Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications

Unit II
Glasses, Ceramics, Composites and Nanomaterials

Unit III
Thin Films and Langmuir-Blodgett Films
Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

Unit IV
Liquid Crystals
Mesomorphic behavior, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic-nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

Unit V
Polymeric Materials
Molecular shape, structure and configuration, crystallinity, stress-strain behavior, thermal behavior, polymer types and their applications, conducting and ferro-electric polymers.

Unit VI
Ionic Conductors
Types of ionic conductors, mechanism of ionic conductors, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

Unit VII
High Tc Materials
Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high Tc materials, applications of high Tc materials.

Books Suggested
7. Inorganic Materials: Recent Advances, Editors D. Bahadur et al., Narosa

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**Unit I**

**General Properties of Liquids**
(a) Liquids as dense gases, liquids as disordered solids, some thermodynamics relations, internal pressure and its significance in liquids. Equations of state, critical constants. Different types of intermolecular forces in liquids, different potential functions for liquids. Additivity of pair potential approximation.
(b) A classical partition function for liquid for liquids, correspondence principle, configuration integral, configuration properties.

**Unit II**

**Theory of Liquids**
Theory of liquids, partition function method or model approach, single cell models, communal energy and entropy, LTD model, significant structure model.

**Unit III**

**Distribution Function and Related Equations**
Radial distribution function method, equation of state in terms of RDF, Molecular distribution functions, pair distribution function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion.

**Unit IV**

**Methods for Structure Determination and Computational Techniques**
Spectroscopic techniques for liquid dynamic structure studies, Neutron and X-ray scattering spectroscopy.
Computation Techniques- Monte Carlo and molecular dynamics methods.

**Unit V**

**Supercooled and Ionic Liquids.**
Supercooled and ionic liquids, theories of transport properties; non Arrhenius behavior of transport properties, Cohen-Turnbull free volume model, configurational entropy model, Macedo-Lltovitz hybrid model, glass transition in supercooled liquids.

**Books Suggested**
2. The Dynamic Liquid State, A.F.M. Barton, Longman.
4. The Liquid State, J.A. Pryde.

**SEMESTER IV**

Inorganic Chemistry

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**Note:** The duration of examination will be of eight hours. Students are required to do two practicals of 30 marks each.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

I. **Spectrophotometric Determinations**
(a). Manganese/chromium/vanadium in steel sample.
(b). Nickle/molybdenum/tungsten/vanadium/uranium by extractive Spectrophotometric method.
(c). Fluoride/nitrite/phosphate.

II. **Flame Photometric Determinations**
(a). Sodium and Potassium when present together.
(b). Lithium/Calcium/barium/strontium.
(c). Cadmium and magnesium in tap water.

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**Note:** The duration of examination will be of eight hours. Students are required to do two practicals of 30 marks each.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

I. **Nephelometric Determinations**
(a). Sulphate
(b). Phosphate
(c). Silver

II. Chromatographic separations: Paper or TLC and determination of Rf values:
(a). Cadmium and Zinc.
(b). Silver, Lead and Mercury.
(c). Nickel, Magnesium, Cobalt and Zinc.

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<th>SOS/C024</th>
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Unit I
Inorganic polymer synthesis, step-growth and step condensation synthesis of metal containing polymers.

Unit II
Condensation of functionalised metal containing species, condensation through bridged ligand coordination, bridging ligand formation during condensation, synthesis of main group condensation polymer.

Unit III
Polycarboranes, polycarbosilanes, polythalocyanines, polysiloxanes.

Unit IV
Chain polymerisations, radical and cationic polymerisations.

Unit V
Inorganic polymer characterization, methods of characterizing average molecular masses.

Unit VI
Glass transition temperature measurement, spectroscopic characterization specific to inorganic polymers, use of NMR and EPR in characterization of inorganic polymers, use of electronic, vibrational, Mossbauer spectroscopies in characterization of inorganic polymers, visco-elasticity measurements. Crystallinity characterization.

Unit VII
Polymer elastomers, inorganic dental polymers, adhesives, inorganic high temperature fluids and lubricants.

Unit VIII
Inorganic polymer conductivity, metal containing polymers, metal containing polymers in non linear optics, luminescent inorganic polymers.

Books suggested
Unit I  
**Electron Spin Resonance Spectroscopy**  
Principle and theory, Kramer degeneracy, g factor, electron-nuclear coupling (hyperfine structure), line shape and width, McConnell relationship, endor and eldor, electron-electron coupling. Techniques of measurement, application of ESR to organic free radicals and to transitional metal complexes (having unpaired electron) including biological systems.

Unit II  
**Mossbauer Spectroscopy**  
Basic principles, spectral parameters and spectrum display. Fine structure, application of the technique to the studies of (1) bonding and structure of Fe$^{2+}$ and Fe$^{3+}$ compounds (2) Sn$^{2+}$ and Sn$^{4+}$ compounds, detection of oxidation state and in equivalent MB atoms.

Unit III  
**Nuclear Magnetic Resonance Spectroscopy**  
(a). Chemical shift values for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, carboxylic acids, amines, amides), chemical exchange, effects of deuteration, Karplus curve-variation of coupling constant with dihedral angle.  
(b). **Carbon-13 NMR Spectroscopy**  
General consideration, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl compound), coupling constants.

Unit IV  
**Mass Spectrometry**  
Principle and theory, fundamental mass equation, ionization methods, odd and even electron ions, base peak, isotopic ions, fragmentation patterns, McLafferty rearrangement and RD cleavage, application of mass spectrometry to the structure elucidation of organic molecules.

Unit V  
**Photoelectron Spectroscopy**  
Basic principles, photoelectric effect, ionization process, Koopman’s Theorem, photoelectron spectra of simple molecules, ESCA, chemical information from ESCA, Auger electron spectroscopy—basic idea.

**Books Suggested**  
Unit I
Bioinorganic Chemistry
1. Electron Transfer in Biology
   Structure and function of metalloproteins in electron transport processes-cytochromes and ion-
sulphur proteins, synthetic models.
2. Nitrogenase
   Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other
   nitrogenases model systems.

Unit II
Bioorganic Chemistry
1. Co-Enzyme Chemistry
   Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and
   biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+
   FMN, FAD, lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.
2. Enzyme Models
   Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry
   and prochirality. Biomimetic chemistry, crown ethers, cryptates. Cyclodextrins, cyclodextrin-based
   enzyme models, calixarenes, ionophores, micelles, synthetic enzymes.
3. Biotechnological Applications of Enzymes
   Large-scale production and purification of enzymes, techniques and methods of immobilization of
   enzymes, use of enzymes in food and drink industry, brewing and cheese-making, syrups from corn
   starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and
   recombinant DNA technology.

Unit III
Biophysical Chemistry
1. Statistical Mechanism in Biopolymers
   Chain configuration of macromolecules, statistical distribution, end-to-end dimensions, calculation
   of average dimensions for various chain structures. Polypeptide and protein structures, introduction
to protein folding problem.
2. Biopolymer Interactions, Thermodynamics of Biopolymer Solutions
   Forces involved in biopolymer interactions. Electrostatic charge and molecular expansion,
   hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding
   processes in biological systems. Thermodynamics of biopolymer solutions, osmotic pressure,
   membrane equilibrium, muscular contraction and energy generation in mechanochemical system.
3. Biopolymers and their Molecular Weights
   Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various
   experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion,
sedimentation velocity, viscosity, electrophoresis and rotational motions.

Books Suggested
4. Understanding Enzymes, Trevor Palmer, Prentice Hall.

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Unit I
Basics of photochemistry

Unit II
Properties of Excited States

Unit III
Excited States of Metal Complexes

Unit IV
Ligand Field Photochemistry
Photosubstitution, photo oxidation and photo reduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.
Unit V
Redox Reactions by Excited Metal Complexes
Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidizing character of Ruthenium\(^{2+}\), (bipyridyl complex, comparison with Fe (bipy)\(_3\)); role of spin-orbit coupling, life time of these complexes. Application of redox processes of electronically excited states for catalytic purpose, transformation of low energy reactants into high-energy products, chemical energy into light.

Unit VI
Metal Complex Sensitizers
Metal complex sensitizer, electron relay, metal colloid system, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

Books Suggested:
10. Introductory Photochemistry, A. Cox
Unit IV
Atmosphere

Unit V
Industrial Pollution
Pollution from cement, sugar, distillery, drug; paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers and drugs etc.

Unit VI
Environmental Toxicology
Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes.

Books suggested

Organic Chemistry

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Note: The duration of examination will be of eight hours. Students are required to do two practicals of 30 marks each.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

I. Extraction of Organic Compounds from Natural Sources
1. Isolation of caffeine from tea leaves.
2. Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).
3. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported).
4. Isolation of nicotine dipicrate from tobacco.
5. Isolation of cinchonine from cinchona bark.
6. Isolation of piperine from black pepper.
7. Isolation of lycopene from tomatoes.
8. Isolation of β-carotene from carrots.
9. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid).
10. Isolation of eugenol from cloves.
11. Isolation of limonene from citrus fruits.

II. Paper Chromatography
Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.

Books Suggested

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Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

I. Spectroscopy
Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS)

II. Spectrophotometric (UV/VIS) Estimations
1. Amino acids
2. Proteins
3. Carbohydrates
4. Cholesterol
5. Ascorbic acid
6. Aspirin
7. Caffeine

Books Suggested
Unit I
Terpenoids and Carotenoids
Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule Structures of abietic acid and β-carotene.

Unit II
Alkaloids
Isolation, structure and synthesis of ephedrine, quinine.

Unit III
Steroids
Structure determination of cholesterol and bile acids (without synthesis). Chemistry of testosterone, estrone and progestrone.

Unit IV
Pigments
(a) Plant Pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of cyanidin, and quercetin.
(b) Porphyrins

Unit V
Prostaglandins
Occurrence, nomenclature, classification, biogenesis and physiological effects
Synthesis of Key intermediate, PGE$_2$ and PGF$_{2α}$

Books Suggested

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Unit I
Nomenclature of Heterocycles
Replacement and Systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles

Unit II
Aromatic and Non-aromatic Heterocycles
General chemical behaviour of aromatic heterocycles, classification (structural type), Heteroaromatic reactivity and tautomerism in aromatic heterocycles
Strain – bond angle and torsional strains and their consequences in small ring heterocycles.
Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interactions.
Stereo-electronic effects, aromatic and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic, electrophilic interactions.

Unit III
Small Ring Heterocycles
Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes

Unit IV
Benzo-Fused Five-Membered Heterocycles
Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes

Unit V
Six-Membered Heterocycles with One, Two or More Heteroatoms
Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones
Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones Synthesis and reactions of diazines, triazines, tetrazines and thiazines

Unit VI
Seven-and Large-Membered Heterocycles
Synthesis and reactions of azepines, oxepines, thiepines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines

Books Suggested
1. Determination of transport number.
2. Determination of liquid junction potential.
3. Determination of the charge on colloidal particle.
4. Polarography.
5. Beer’s law verification.

Note: The duration of examination will be of eight hours. Students are required to do one practical of 60 marks.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.

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<td>100</td>
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1. Decomposition of potential determination.
2. Validity of Freundlich’s adsorption isotherm.
5. Determination of CMC of surfactants.

Note: The duration of examination will be of eight hours. Students are required to do one practical of 60 marks.
Viva 15 marks
Seminar/Attendance/Assessment/Record 25 marks.
(Pre-requisite: mathematics at least up to First Year B.Sc. level is necessary. At least one PC among 4 students should be available)

**Unit I**
**Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock Theory**
Review of the principles of quantum mechanics, Born-Oppenheimer approximation. Slater-Condon rules, Hartree-Fock equation, Koopmans and Brillouin theories, Roothan equation, Gaussian basis sets.

**Unit II**
**Configuration Interaction and MC-SCF**
Introduction to CI; full and truncated CI theories, size consistency, Introductory treatment of coupled cluster and MC-SCF methods.

**Unit III**
**Semi-Empirical Theories**

**Unit IV**
**Density Functional Theory**
Derivation of Hohenberg-Kohn theorem, Kohn-Sham formulation, N- and V- representabilities; review of the performance of the existing local (e.g. Slater Xa and other methods) and non-local functionals, treatment of chemical concepts with the density functional theory.

**Unit V**
**Computer Experiments**
Computer experiments using quantum chemistry- software packages such as GAUSSIAN/GAMESS/MOPAC and modeling software e.g. MM2/ AMBER/ CHARM etc.

**Books Suggested**
Unit I
Basics

Unit II
Polymer Characterization

Unit III
Structure and Properties
Morphology and order in crystalline polymers, configurations of polymer chains. Crystal structure of polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties, crystalline melting point Tm, melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg. Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

Unit IV
Polymer Processing

Books Suggested

Self Study Courses in Chemistry

1. Computers for Chemists Credits 3 MM 100
This is a theory-cum-laboratory course with more emphasis on laboratory work.

I Introduction to Computers and Computing
Computer fundamentals, Classification of Digital computers: PC, Microcomputers, minicomputers, mainframe computers, supercomputers, MIDI.  
Number Systems: Binary, Decimal, Hexadecimal and Octal number systems and their conversion from one system to another system. Boolean Algebra and logic gates. Character codes ASCII & EBCDIC. 
Basic architecture of the Computer, Input & output Devices, CPU, Processor, Memory. Temporary and Permanent Memory; ROM, RAM, Cache Memory.  

II C & C++ Languages
Computer languages.  
Programming in C: Variables, expressions, assignments and data types, preprocessors. Use of printf() and scanf(). 
Arithmetic operators, comparison operators, logical operators, precedence among different types of operators, parenthesis. 
Selection constructs: IF Constructs, If...Else constructs, Multiple criteria using AND and OR, DO CASE. 
Loops: the WHILE loop, the DO. . . . While loop, REPEAT.. UNTIL loop, FOR loop. 
Functions, procedures, function libraries, Elementary idea of Arrays, strings and structures. 
Computer graphics: Graphic types. SCREEN. Displaying a point. Drawing of Line, Box, Circle and Ellipse. 
Drawing non-geometric shapes with DRAW statements. WINDOW, VIEW, PAINT statements.

III Programming in Chemistry
Development of small computer codes involving simple formulae in chemistry, such as van der Waals Equation pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge database. 
Matrix algebra- Matrix, Matrix type, Matrix operators, Matrix representation, Addition/Subtraction/Multiplications/Transpose of Matrices. 

IV Use of Computer Programmes
The student will learn to operate a PC and to run standard programs and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programs. Monte Carlo and Molecular dynamics. Programs with data preferably from physical chemistry laboratory. Further, the students will operate one or two of the packages such as MATLAB / SCILAB, EASYPLOT/ GNUPLOT, FOXPRO/ MYSQL, MSOFFICE / OPENOFFICE. 
Working with Internet and email. 
Working with UNIX/ LINUX/ DOS/ WINDOWS OS: Creating Folder, Shortcuts, Creating text files, Finding Files, Renaming and deleting file or folder, working with recycle bin / trash bin, setting desktop wallpaper, screen savers, shutting down. Copying Folders and files.
Working with Word processors, creating a document, editing, formatting text and paragraphs, moving and copying text, headers and footers, setting and and tabs. Viewing document windows, working with columns, save and protect documents, working with tables.

Working with spreadsheets, creating workbooks and worksheets, working with numbers, modifying the worksheet layout, printing worksheets, formatting worksheets, selecting multiple cells, writing simple formulae, writing complex formulae, copying and editing formulae, formatting the cell, moving and copying cell, formatting rows and columns, using excel for data base management, cell referencing, relative and absolute referencing, introduction to charts, creating charts, editing and formatting charts, printing the graphs, using cell references in conditions, using formulae in conditions.

Working with databases, file creation, modifying a file, adding records, selecting records, and printing reports.

Books Suggested
3. A Handbook of MS Office.
4. Programming in C: E. Balaguruswamy, TMH
7. Microcomputer Quantum Mechanics: J.P. Killingbeck, Adam Hinger

2. Mathematics for Chemists Credits 3 MM 100
(For students without Mathematics in B.Sc.)

I. Vectors and Matrix Algebra
A. Vectors
Vectors, dot, cross and triple products etc. The gradient, divergence and curl. Vector calculus, Gauss’ theorem, divergence theorem etc.

B. Matrix Algebra
Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (symmetric, skew-symmetric, Hermitian, skew-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence. Introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants (examples from Huckel theory). Introduction to tensors; polarizability and magnetic susceptibility as examples.

II. Differential Calculus
Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr’s radius and most probable velocity from Maxwell’s distribution etc.), exact and inexact differentials with their applications to thermodynamic properties. Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate, transformations (e.g. cartesian to spherical polar), curve sketching.
III. Elementary Differential Equations
Variables-separable and exact first-order differential equations, homogeneous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. Solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and Legendre equation etc., spherical harmonics, second order differential equations and their solutions.

IV. Permutation and Probability
Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, examples from the kinetic theory of gases etc. curve fitting (including least squares fit etc.) with a general polynomial fit.

Books Suggested

3. Nanoscience and Nanotechnology Credits 3 MM 100

Unit I
Introduction
Historical perspective of nano, nanoscience, nano and nature, shift from micro to nano, quantum size effects.

Unit II
Diversity in nanosystems
Carbon nanoscience (fullerenes and nanotubes), nanowires, nanorods, self assembled monolayers (SAMS).

Unit III
Characterization of nanomaterials
Instrumentation for the characterization of nanomaterials. Principle and applications of various techniques.

Unit IV
Interdisciplinary nature of nanoscience
Smart materials-nanobiology, nanosensors, nanomedicines, nanotribology, molecular electronics (nanomachines).

Unit V
Nano and society
Implications of nano-science and technology on society, nanorelated issues, nanopolicies and institutions, public involvement in nanodiscourse, nanotechnology for social and economic development.
Books Suggested