

# **CHOICE BASED CREDIT SYSTEM**

## **B. Sc. WITH CHEMISTRY**

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

Course	*Credits	
	Theory+ Practical	Theory+Tutorials
<b><u>I. Core Course</u></b>	12×4= 48	12×5=60
<b>(12 Papers)</b>		
04 Courses from each of the 03 disciplines of choice		
<b>Core Course Practical / Tutorial*</b>	12×2=24	12×1=12
<b>(12 Practical/ Tutorials*)</b>		
04 Courses from each of the 03 Disciplines of choice		
<b><u>II. Elective Course</u></b>	6×4=24	6×5=30
<b>(6 Papers)</b>		
Two papers from each discipline of choice including paper of interdisciplinary nature.		
<b>Elective Course Practical / Tutorials*</b>	6×2=12	6×1=6
<b>(6 Practical / Tutorials*)</b>		
Two Papers from each discipline of choice including paper of interdisciplinary nature		
<ul style="list-style-type: none"> <li>• <b>Optional Dissertation or project work in place of one Discipline elective paper (6 credits) in 6<sup>th</sup> Semester</b></li> </ul>		

**III. Ability Enhancement Courses**

1. **Ability Enhancement Compulsory**                      2×2=4    2×2=4

**(2 Papers of 2 credits each)**

**Environmental Science**

**English/MIL Communication**

2. **Skill Enhancement Course**    4×2=8    4×2=8

**(Skill Based)**

**(4 Papers of 2 credits each)**

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**Total credit= 120**

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**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**

	<b>CORE COURSE (12)</b>	<b>Ability Enhancement Compulsory Course (AECC) (2)</b>	<b>Skill Enhancement Course (SEC) (2)</b>	<b>Discipline Specific Elective DSE (6)</b>
I	DSC- 1 A	(English /MIL Communication)/ Environmental Science		
	Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons			
	DSC- 3 A			
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			
IV	DSC- 1 D		SEC -2	
	Transition Metal & Coordination chemistry, States of Matter & Chemical Kinetics			
	DSC- 3 D			
V			SEC -3	DSE-1 A
				DSE-2 A
				DSE-3 A
VI			SEC -4	DSE-1 B
				DSE-2 B
				DSE-3 B

<b>SEMESTER</b>	<b>COURSE OPTED</b>	<b>COURSE NAME</b>	<b>Credits</b>
<b>I</b>	<b>Ability Enhancement Compulsory Course-I</b>	<b>English/MIL communications/ Environmental Science</b>	<b>2</b>
	<b>Core Course-I</b>	<b>DSC 1A</b>	<b>6</b>
	<b>Core Course-II</b>	<b>Atomic Structure, Bonding, General Organic Chemistry &amp; Aliphatic Hydrocarbons</b>	<b>4</b>
	<b>Core Course-II Practical/ Tutorial</b>	<b>Atomic Structure, Bonding, General Organic Chemistry &amp; Aliphatic Hydrocarbons Lab</b>	<b>2</b>
	<b>Core Course-III</b>	<b>DSC 3A</b>	<b>6</b>
<b>II</b>	<b>Ability Enhancement Compulsory Course-II</b>	<b>English/MIL communications/ Environmental Science</b>	<b>2</b>
	<b>Core Course-IV</b>	<b>DSC 1B</b>	<b>6</b>
	<b>Core Course-V</b>	<b>Chemical Energetics, Equilibria &amp; Functional Group Organic Chemistry-I</b>	<b>4</b>
	<b>Core Course-V Practical/ Tutorial</b>	<b>Chemical Energetics, Equilibria &amp; Functional Group Organic Chemistry-I Lab</b>	<b>2</b>
	<b>Core Course-VI</b>	<b>DSC 3B</b>	<b>6</b>
<b>III</b>	<b>Core Course-VII</b>	<b>DSC 1C</b>	<b>6</b>
	<b>Core Course-VIII</b>	<b>Solutions, Phase Equilibria, Conductance, Electrochemistry &amp; Functional Group Organic Chemistry-II</b>	<b>4</b>
	<b>Core Course-VIII Practical/ Tutorial</b>	<b>Solutions, Phase Equilibria, Conductance, Electrochemistry &amp; Functional Group Organic Chemistry-II Lab.</b>	<b>2</b>
	<b>Core Course-IX</b>	<b>DSC 3C</b>	<b>6</b>
	<b>Skill Enhancement Course -1</b>	<b>SEC-1</b>	<b>2</b>
<b>IV</b>	<b>Core Course-X</b>	<b>DSC 1D</b>	<b>6</b>
	<b>Core Course-XI</b>	<b>Transition Metal &amp; Coordination chemistry, States of matter &amp; Chemical kinetics</b>	<b>4</b>
	<b>Course-XI Practical/Tutorial</b>	<b>Transition Metal &amp; Coordination chemistry, States of matter &amp; Chemical kinetics Lab</b>	<b>2</b>
	<b>Core Course-XII</b>	<b>DSC 3D</b>	<b>6</b>
	<b>Skill Enhancement Course -2</b>	<b>SEC-2</b>	<b>2</b>
<b>V</b>	<b>Skill Enhancement Course -3</b>	<b>SEC-3</b>	<b>2</b>
	<b>Discipline Specific Elective -1</b>	<b>DSE-1A</b>	<b>6</b>
	<b>Discipline Specific Elective -2</b>	<b>DSE-2A</b>	<b>6</b>
	<b>Discipline Specific Elective -3</b>	<b>DSE-3A</b>	<b>6</b>

<b>VI</b>	<b>Skill Enhancement Course -4</b>	<b>SEC-4</b>	<b>2</b>
	<b>Discipline Specific Elective -4</b>	<b>DSE-1B</b>	<b>6</b>
	<b>Discipline Specific Elective -5</b>	<b>DSE-2B</b>	<b>6</b>
	<b>Discipline Specific Elective-6</b>	<b>DSE-3B</b>	<b>6</b>
<b>Total Credits</b>			<b>120</b>

## **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)
3. Conductance, Electrochemistry & Functional Group Organic Chemistry-II (4) + Lab (4)
4. Transition Metal & Coordination chemistry, States of Matter and Chemical Kinetics (4) + Lab (4)

### **Discipline Specific Elective papers (Credit: 06 each) (DSE 1, DSE 2): Choose2**

#### **Chemistry**

1. Analytical Methods in Chemistry (4) + Lab (4)
2. Industrial Chemicals & Environment (4) + Lab (4)
3. Instrumental Methods of Analysis (4) + Lab (4)
4. Quantum Chemistry, Spectroscopy & Photochemistry (4) + Lab (4)
5. *Chemistry of Main Group Elements, Theories of Acids and Bases.*

### **Skill Enhancement Course (any four) (Credit: 02 each) - SEC 1 to SEC 4**

#### **Chemistry**

1. Basic Analytical Chemistry
2. Chemoinformatics
3. Green Methods in Chemistry
4. Pharmaceutical Chemistry
5. Pesticide Chemistry
6. Fuel Chemistry

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## Semester I

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### CHEMISTRY-DSC 2A: ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

#### *Section A: Inorganic Chemistry-1 (30 Periods)*

**Atomic Structure:** Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure.

What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of  $\psi$  and  $\psi^2$ , Schrödinger equation for hydrogen atom. Radial and angular parts of the hydrogenic 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<sup>+</sup>. Comparison of VB and MO approaches.

(16 Lectures)

### **Section B: Organic Chemistry-I (30 Periods)**

#### **Fundamentals of Organic Chemistry**

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis.

Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals.

Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule.

(8 Lectures)

#### **Stereochemistry**

Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations. Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; *cis-trans* nomenclature; CIP Rules: R/S (for upto 2 chiral carbon atoms) and E/Z Nomenclature (for upto two C=C systems).

(10 Lectures)

#### **Aliphatic Hydrocarbons**

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

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

**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. KMnO<sub>4</sub>) 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<sub>2</sub> 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  $\text{KMnO}_4$ , ozonolysis and oxidation with hot alk.  $\text{KMnO}_4$ .

(12 Lectures)

**Reference Books:**

- Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
- Cotton, F.A., Wilkinson, G. & Gaus, P.L. *Basic Inorganic Chemistry*, 3<sup>rd</sup> ed., Wiley.
- Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*, John Wiley & Sons.
- Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Education India, 2006.
- Graham Solomon, T.W., Fryhle, C.B. & Snyder, S.A. *Organic Chemistry*, John Wiley & Sons (2014).
- McMurry, J.E. *Fundamentals of Organic Chemistry*, 7<sup>th</sup> Ed. Cengage Learning India Edition, 2013.
- Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).
- Eliel, E.L. *Stereochemistry of Carbon Compounds*, Tata McGraw Hill education, 2000.
- Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.
- Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.
- Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.

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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  $\text{KMnO}_4$ .
3. Estimation of water of crystallization in Mohr's salt by titrating with  $\text{KMnO}_4$ .
4. Estimation of Fe (II) ions by titrating it with  $\text{K}_2\text{Cr}_2\text{O}_7$  using internal indicator.
5. Estimation of Cu (II) ions iodometrically using  $\text{Na}_2\text{S}_2\text{O}_3$ .

***Section B: Organic Chemistry***

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)
2. Separation of mixtures by Chromatography: Measure the  $R_f$  value in each case (combination of two compounds to be given)

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

**Reference Books:**

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.

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**Semester II**

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**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  $G$  and  $G^\circ$ , 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.

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

**(8 Lectures)**

### **Alkyl and Aryl Halides**

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

*Preparation:* from alkenes and alcohols.

*Reactions:* hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis: Elimination vs substitution.

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

*Reactions (Chlorobenzene):* Aromatic nucleophilic substitution (replacement by  $-OH$  group) and effect of nitro substituent. Benzyne Mechanism:  $KNH_2/NH_3$  (or  $NaNH_2/NH_3$ ).

Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

**(8 Lectures)**

### **Alcohols, Phenols and Ethers (Upto 5 Carbons)**

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

*Reactions:* With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. KMnO<sub>4</sub>, acidic dichromate, conc. HNO<sub>3</sub>). Oppeneauer oxidation *Diols:* (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement.

**Phenols:** (Phenol case) *Preparation:* Cumene hydroperoxide method, from diazonium salts. *Reactions:* Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben-Hoesch Condensation, Schotten – Baumann Reaction.

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

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

*Preparation:* from acid chlorides and from nitriles.

*Reactions* – Reaction with HCN, ROH, NaHSO<sub>3</sub>, NH<sub>2</sub> -G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Ponndorf Verley reduction.

(14 Lectures)

#### Reference Books:

- Graham Solomon, T.W., Fryhle, C.B. & Snyder, S.A. *Organic Chemistry*, John Wiley & Sons (2014).
- McMurry, J.E. *Fundamentals of Organic Chemistry*, 7<sup>th</sup> Ed. Cengage Learning India Edition, 2013.
- Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).
- Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.
- Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.
- Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.
- Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
- Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
- Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
- Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).

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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 (KNO<sub>3</sub>, NH<sub>4</sub>Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of *H*.
7. Determination of solubility product.

### **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**

- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
  - Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.
  - Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
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### Semester III

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## **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**

Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions. Vapour pressure-composition and temperature-composition curves of ideal and non-ideal solutions. Distillation of solutions. Lever rule. Azeotropes.

Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Immiscibility of liquids- Principle of steam distillation. Nernst distribution law and its applications, solvent extraction.

**(8 Lectures)**

#### **Phase Equilibrium**

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

**(8 Lectures)**

#### **Conductance**

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions.

Transference number and its experimental determination using Hittorf and Moving boundary methods. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid-base).

**(6 Lectures)**

#### **Electrochemistry**

Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties:  $G$ ,  $H$  and  $S$  from EMF data.

Calculation of equilibrium constant from EMF data. Concentration cells with transference and without transference. Liquid junction potential and salt bridge.

pH determination using hydrogen electrode and quinhydrone electrode.

Potentiometric titrations -qualitative treatment (acid-base and oxidation-reduction only).

**(8 Lectures)**

### ***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.

*Reactions:* Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

**(6 Lectures)**

#### **Amines and Diazonium Salts**

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

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

*Reactions:* Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with  $\text{HNO}_2$ , Schotten – Baumann Reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation.

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



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

(6 Lectures)

### **Amino Acids, Peptides and Proteins:**

*Preparation of Amino Acids:* Strecker synthesis using Gabriel's phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis.

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

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

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

(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 disaccharides (sucrose, cellobiose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

(8 Lectures)

### **Reference Books:**

- Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
  - Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
  - Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry*, Cengage Learning India Pvt. Ltd.: New Delhi (2009).
  - Mahan, B.H. *University Chemistry*, 3rd Ed. Narosa (1998).
  - Petrucci, R.H. *General Chemistry*, 5th Ed., Macmillan Publishing Co.: New York (1985).
  - Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
  - Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
  - Finar, I. L. *Organic Chemistry (Volume 2)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
  - Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Biochemistry 7<sup>th</sup> Ed.*, W. H. Freeman.
  - Berg, J.M., Tymoczko, J.L. & Stryer, L. *Biochemistry*, W.H. Freeman, 2002.
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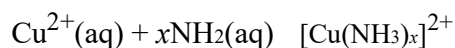
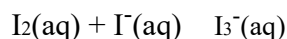
# CHEMISTRY LAB-DSC 2C LAB: SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY & FUNCTIONAL ORGANIC CHEMISTRY-II

60 Lectures

## Section A: Physical Chemistry

### Distribution

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



2. Partition co-efficient

### Phase equilibria

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

### Conductance

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

### Viscosity

- Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwalds' viscometer

### Potentiometry

Perform the following potentiometric titrations:

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

## ***Section B: Organic Chemistry***

**I** Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (-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 and a nonreducing sugar.

### **Reference Books:**

- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
  - Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.
  - Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
  - Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.
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## Semester IV

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### **CHEMISTRY-DSC 2D: TRANSITION METAL & COORDINATION CHEMISTRY, STATES OF MATTER & CHEMICAL KINETICS**

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

**Theory: 60 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**

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

Drawbacks of VBT. IUPAC system of nomenclature.

**(8 Lectures)**

#### **Crystal Field Theory**

Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of D. Spectrochemical series. Comparison of CFSE for  $O_h$  and  $T_d$  complexes, Tetragonal distortion of octahedral geometry.

Jahn-Teller distortion, Square planar coordination.

**(10 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<sub>2</sub>.

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).

**(8 Lectures)**

### **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).

**(6 Lectures)**

### **Solids**

Forms of solids. Symmetry elements, unit cells, crystal systems, Bravais lattice types and identification of lattice planes. Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices. Miller indices. X-Ray diffraction by crystals, Bragg's law. Structures of NaCl, KCl and CsCl (qualitative treatment only). Defects in crystals. Glasses and liquid crystals.

**(8 Lectures)**

### **Chemical Kinetics**

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

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

**(8 Lectures)**

**Reference Books:**

- Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
- Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
- Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
- Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
- Cotton, F.A. & Wilkinson, G. *Basic Inorganic Chemistry*, Wiley.
- Shriver, D.F. & Atkins, P.W. *Inorganic Chemistry*, Oxford University Press.
- Wulfsberg, G. *Inorganic Chemistry*, Viva Books Pvt. Ltd.
- Rodgers, G.E. *Inorganic & Solid State Chemistry*, Cengage Learning India Ltd., 2008.

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**CHEMISTRY LAB-DSC 2D LAB: TRANSITION METAL & COORDINATION CHEMISTRY, STATES OF MATTER & CHEMICAL KINETICS**

**60 Lectures**

***Section A: Inorganic Chemistry***

Semi-micro qualitative analysis using H<sub>2</sub>S of mixtures - not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations : NH<sub>4</sub><sup>+</sup>, Pb<sup>2+</sup>, Ag<sup>+</sup>, Bi<sup>3+</sup>, Cu<sup>2+</sup>, Cd<sup>2+</sup>, Sn<sup>2+</sup>, Fe<sup>3+</sup>, Al<sup>3+</sup>, Co<sup>2+</sup>, Cr<sup>3+</sup>, Ni<sup>2+</sup>, Mn<sup>2+</sup>, Zn<sup>2+</sup>, Ba<sup>2+</sup>, Sr<sup>2+</sup>, Ca<sup>2+</sup>, K<sup>+</sup>

Anions : CO<sub>3</sub><sup>2-</sup>, S<sup>2-</sup>, SO<sub>3</sub><sup>2-</sup>, S<sub>2</sub>O<sub>3</sub><sup>2-</sup>, NO<sub>3</sub><sup>-</sup>, CH<sub>3</sub>COO<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, NO<sub>2</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, PO<sub>4</sub><sup>3-</sup>, BO<sub>3</sub><sup>3-</sup>, C<sub>2</sub>O<sub>4</sub><sup>2-</sup>, F<sup>-</sup>

*(Spot tests should be carried out wherever feasible)*

1. Estimate the amount of nickel present in a given solution as bis(dimethylglyoximate) nickel(II) or aluminium as oximate in a given solution gravimetrically.
2. Estimation of (i) Mg<sup>2+</sup> or (ii) Zn<sup>2+</sup> by complexometric titrations using EDTA.
3. Estimation of total hardness of a given sample of water by complexometric titration.

## ***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.

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

- a) 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<sub>2</sub>SO<sub>4</sub> by studying kinetics of hydrolysis of methyl acetate

### **Reference Books:**

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
  - Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
  - Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
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**Discipline Specific Electives**  
**Select two papers**

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**--- CHEMISTRY-DSE I-IV (ELECTIVES)**

**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:**

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

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

*Basic principles of quantitative analysis:* estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.

*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:

- Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. *Vogel's Textbook of Quantitative Chemical Analysis*, John Wiley & Sons, 1989.
- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*, 7<sup>th</sup> Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.
- Christian, G.D; *Analytical Chemistry*, 6<sup>th</sup> Ed. John Wiley & Sons, New York, 2004.
- Harris, D. C. *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.
- Mikes, O. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.
- Ditts, R.V. *Analytical Chemistry; Methods of Separation*, van Nostrand, 1974.

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## PRACTICALS- DSE LAB: ANALYTICAL METHODS IN CHEMISTRY

### 60 Lectures

#### I. Separation Techniques

##### 1. Chromatography:

##### (a) Separation of mixtures

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

(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:

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

2. 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.

### **BI 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:**

- Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. *Vogel's Textbook of Quantitative Chemical Analysis*, John Wiley & Sons, 1989.
- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*, 7<sup>th</sup> Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.
- Christian, Gary D; *Analytical Chemistry*, 6<sup>th</sup> Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.

- Mikes, O. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.
- Ditts, R.V. *Analytical Chemistry; Methods of Separation*, van Nostrand, 1974.

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## CHEMISTRY-DSE: INDUSTRIAL CHEMICALS AND ENVIRONMENT

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**(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**

#### **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.

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

**(8 Lectures)**

## **Environment and its segments**

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution.

Pollution by SO<sub>2</sub>, CO<sub>2</sub>, CO, NO<sub>x</sub>, H<sub>2</sub>S and other foul smelling gases. Methods of estimation of CO, NO<sub>x</sub>, SO<sub>x</sub> 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:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
  - R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
  - J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
  - S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
  - K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
  - S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi
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- S.E. Manahan, *Environmental Chemistry*, CRC Press (2005).
  - G.T. Miller, *Environmental Science* 11th edition. Brooks/ Cole (2006).
  - A. Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).
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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 ( $\text{AgNO}_3$  and potassium chromate).
6. Estimation of total alkalinity of water samples ( $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$ ) using double titration method.
7. Measurement of dissolved  $\text{CO}_2$ .
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

### Reference Books:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
  - R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
  - J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
  - S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
  - K. De, *Environmental Chemistry*: New Age International Pvt. Ltd, New Delhi.
  - S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
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## **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 spectroscopy:* Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation).

(16 Lectures)

### **Elemental analysis:**

Mass spectrometry (electrical discharges).

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

(4 Lectures)

**Radiochemical Methods**

(4 Lectures)

**X-ray analysis and electron spectroscopy (surface analysis)**

(4 Lectures)

### **Reference books:**

- Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.
- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*, 7<sup>th</sup> Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.
- P.W. Atkins: Physical Chemistry.
- G.W. Castellan: Physical Chemistry.
- C.N. Banwell: Fundamentals of Molecular Spectroscopy.
- Brian Smith: Infrared Spectral Interpretations: A Systematic Approach.
- W.J. Moore: Physical Chemistry.



**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:**

- Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.
- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*, 7<sup>th</sup> Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.

## **DSE: QUANTUM CHEMISTRY, SPECTROSCOPY & PHOTOCHEMISTRY**

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

**Theory: 60 Lectures**

### **Quantum Chemistry**

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

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

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component.

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus.

Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of  $H_2^+$ . Bonding and antibonding orbitals. Qualitative extension to  $H_2$ . Comparison of LCAO-MO and VB treatments of  $H_2$  (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic ( $BeH_2$ ,  $H_2O$ ) molecules. Qualitative MO theory and its application to  $AH_2$  type molecules.

**(24 Lectures)**

## **Molecular Spectroscopy:**

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

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

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

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

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

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules.

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

**(24 Lectures)**

## **Photochemistry**

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

**(12 Lectures)**

## Reference Books:

- Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4<sup>th</sup> Ed. Tata McGraw-Hill: New Delhi (2006).
- Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill (2001).
- House, J. E. *Fundamentals of Quantum Chemistry* 2<sup>nd</sup> Ed. Elsevier: USA (2004).
- Lowe, J. P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).
- Kakkar, R. *Atomic & Molecular Spectroscopy: Concepts & Applications*, Cambridge University Press (2015).

## DSE LAB

### 60 Lectures

#### UV/Visible spectroscopy

- I. Study the 200- 500 nm absorbance spectra of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  (in 0.1 M  $\text{H}_2\text{SO}_4$ ) and determine the  $\lambda_{\text{max}}$  values. Calculate the energies of the two transitions in different units ( $\text{J molecule}^{-1}$ ,  $\text{kJ mol}^{-1}$ ,  $\text{cm}^{-1}$ , eV).
- AI. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of  $\text{K}_2\text{Cr}_2\text{O}_7$ .
- BI. 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  $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$  in a solution of unknown concentration
- AI. Determine the concentrations of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  in a mixture.
- BI. Study the kinetics of iodination of propanone in acidic medium.
- IV. Determine the amount of iron present in a sample using 1,10-phenanthroline.
- V. Determine the dissociation constant of an indicator (phenolphthalein).
- VI. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.
- VII. Analyse the given vibration-rotation spectrum of  $\text{HCl}(\text{g})$

## Reference Books

- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
  - Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
  - Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry* 8<sup>th</sup> Ed.; McGraw-Hill: New York (2003).
  - Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry* 3<sup>rd</sup> Ed.; W.H. Freeman & Co.: New York (2003).
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## CHEMISTRY-DSE: CHEMISTRY OF MAIN GROUP ELEMENTS, THEORIES OF ACIDS AND BASES

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

### Acids and Bases

Brønsted-Lowry concept, conjugate acids and bases, relative strengths of acids and bases, effects of substituent and solvent, differentiating and levelling solvents. Lewis acid-base concept, classification of Lewis acids and bases, Lux-Flood concept and solvent system concept. Hard and soft acids and bases (HSAB concept), applications of HSAB process.

(10 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 and carbon monoxide as reducing agents.

Hydrometallurgy with reference to cyanide process for gold and silver. Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn, Au): electrolytic refining, zone refining, van Arkel-de Boer process, Parting Process, Mond's process and Kroll Process.

(8 Lectures)

### s- and p-Block Elements

Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electron gain enthalpy, electronegativity (Pauling scale). General characteristics of s-block metals like density, melting and boiling points, flame colour and reducing nature. Oxidation states of s- and p-block elements, inert-pair effect, diagonal relationships and anomalous behaviour of first member of each group. Allotropy in C, P and S. Complex forming tendency of s block elements and a preliminary idea of crown ethers and cryptates, structures of basic beryllium acetate, salicylaldehyde/ acetylacetonato complexes of Group 1 metals. Solutions of alkali metals in liquid ammonia and their properties. Common features, such as ease of formation, solubility and stability of oxides, peroxides, superoxides, sulphates and carbonates of s-block metals.

(14 Lectures)

Structure, bonding and properties (acidic/ basic nature, oxidizing/ reducing nature and hydrolysis of the following compounds and their applications in industrial and environmental chemistry wherever applicable:

Diborane and concept of multicentre bonding, hydrides of Groups 13 ( $BH_3$ ), 14, 15, 16 and 17.

Oxides of N and P, Oxoacids of P, S and Cl.

Halides and oxohalides of P and S ( $PCl_3$ ,  $PCl_5$ ,  $SOCl_2$  and  $SO_2Cl_2$ )

Interhalogen compounds.

*A brief idea of pseudohalides*

*(14 Lectures)*

### *Noble gases*

*Rationalization of inertness of noble gases, clathrates, preparation and properties of  $\text{XeF}_2$ ,  $\text{XeF}_4$  and  $\text{XeF}_6$  bonding in these compounds using VBT and shapes of noble gas compounds using VSEPR Theory*

*(5 Lectures)*

### *Inorganic Polymers*

*Types of inorganic polymers and comparison with organic polymers, structural features, classification and important applications of silicates. Synthesis, structural features and applications of silicones. Borazines and cyclophosphazenes - preparation, properties and reactions. Bonding in  $(\text{N}(\text{PCl}_2)_3)_n$ .*

*(9 Lectures)*

### *Recommended texts:*

- Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
- Cotton, F.A., Wilkinson, G. & Gaus, P.L. *Basic Inorganic Chemistry*, 3rd ed., Wiley.
- Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*, John Wiley & Sons.
- Greenwood, N.N. & Earnshaw. *Chemistry of the Elements*, Butterworth-Heinemann, 1997.
- Rodger, G.E. *Inorganic and Solid State Chemistry*, Cengage Learning India Edition, 2002.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry* 4th Ed., Pearson, 2010.
- Atkin, P. Shriver & Atkins' *Inorganic Chemistry* 5th Ed. Oxford University Press (2010).

## **CHEMISTRY PRACTICAL- DSE LAB**

### *60 Periods*

1. Iodometric estimation of potassium dichromate and copper sulphate
2. Iodometric estimation of antimony in tartaremetic
3. Estimation of amount of available chlorine in bleaching powder and household bleaches
4. Estimation of iodine in iodized salts.
5. Iodometric estimation of ascorbic acid in fruit juices.
6. Estimation of dissolved oxygen in water samples.
7. Gravimetric estimation of sulphate as barium sulphate.
8. Gravimetric estimation of aluminium as oximate complex
9. Preparation of the following: potash alum, chrome alum, tetraamminecopper(II) sulphate monohydrate, potassium trioxalatoferrate(III) (any two, including one double salt and one complex).

### *Recommended Texts:*

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.

## Skill Enhancement Course (any four) (Credit: 02 each)- SEC1 to SEC4

### Chemistry

#### 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 ( $\text{Fe}^{3+}$  and  $\text{Al}^{3+}$ ).
- 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:**

- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*. 7<sup>th</sup> Ed. Wadsworth Publishing Co. Ltd., Belmont, California, USA, 1988.
  - Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.
  - Skoog, D.A.; West, D.M. & Holler, F.J. *Fundamentals of Analytical Chemistry* 6<sup>th</sup> Ed., Saunders College Publishing, Fort Worth (1992).
  - Harris, D. C. *Quantitative Chemical Analysis*, W. H. Freeman.
  - Dean, J. A. *Analytical Chemistry Notebook*, McGraw Hill.
  - Day, R. A. & Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India.
  - Freifelder, D. *Physical Biochemistry* 2<sup>nd</sup> Ed., W.H. Freeman and Co., N.Y. USA (1982).
  - Cooper, T.G. *The Tools of Biochemistry*, John Wiley and Sons, N.Y. USA. 16 (1977).
  - Vogel, A. I. *Vogel's Qualitative Inorganic Analysis* 7<sup>th</sup> Ed., Prentice Hall.
  - Vogel, A. I. *Vogel's Quantitative Chemical Analysis* 6<sup>th</sup> Ed., Prentice Hall.
  - Robinson, J.W. *Undergraduate Instrumental Analysis* 5<sup>th</sup> Ed., Marcel Dekker, Inc., New York (1995).
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## 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:

- Andrew R. Leach & Valerie, J. Gillet (2007) *An introduction to Chemoinformatics*. Springer: The Netherlands.
  - Gasteiger, J. & Engel, T. (2003) *Chemoinformatics: A text-book*. Wiley-VCH.
  - Gupta, S. P. (2011) *QSAR & Molecular Modeling*. Anamaya Pub.: New Delhi.
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## GREEN METHODS IN CHEMISTRY

(Credits: 02)

Theory: 30 Lectures

### *Theory and Hand-on Experiments*

Introduction: Definitions of Green Chemistry. Brief introduction of twelve principles of Green Chemistry, with examples, special emphasis on atom economy, reducing toxicity, green solvents, Green Chemistry and catalysis and alternative sources of energy, Green energy and sustainability

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

- Surfactants for carbon dioxide – Replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.
- Designing of environmentally safe marine antifoulant.
- Rightfit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments.
- An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.

### **Practicals**

- Preparation and characterization of biodiesel from vegetable oil.
- Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice.
- Mechano chemical solvent free synthesis of azomethine.
- Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II).

### **Reference Books:**

- Anastas, P.T. & Warner, J.K. *Green Chemistry- Theory and Practical*, Oxford University Press (1998).
- Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker (2001).
- Cann, M.C. & Connely, M.E. *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).
- Ryan, M.A. & Tinnesand, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).
- Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. *Green Chemistry Experiments: A monograph* I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore.
- Lancaster, M. *Green Chemistry: An introductory text* RSC publishing, 2nd Edition.
- Sidhwani, I.T., Saini, G., Chowdhury, S., Garg, D., Malovika, Garg, N. Wealth from waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated “*A Social Awareness Project*”, *Delhi University Journal of Undergraduate Research and Innovation*, **1(1)**: 2015.

## 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:

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

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

### **Reference Book:**

- Cremlyn, R. *Pesticides. Preparation and Modes of Action*, John Wiley & Sons, New York, 1978.
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## **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, pour point) and their determination.

**Reference Books:**

- Stocchi, E. *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK (1990).
  - Jain, P.C. & Jain, M. *Engineering Chemistry* Dhanpat Rai & Sons, Delhi.
  - Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut (1996).
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