

## BSc. Physical Sciences

### DISCIPLINE SPECIFIC CORE COURSE (DSC-1): Basic Concepts of Organic Chemistry

#### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Basic Concepts of Organic Chemistry	04	02	-	02	12 <sup>th</sup> Pass	NIL

#### Learning Objectives

The Learning Objectives of this course are as follows:

- The course is infused with the recapitulation of fundamentals of organic chemistry and the introduction of the concept of visualizing the organic molecules in a three-dimensional space.
- To establish the applications of these concepts, a study of diverse reactions through mechanisms is included.
- The constitution of the course strongly aids in the paramount learning of the basic concepts and their applications

#### Learning outcomes

The Learning Outcomes of this course are as follows:

- Understand and explain the differential behavior of organic compounds based on fundamental concepts learned.
- Understand the fundamental concepts of stereochemistry.
- Formulate the mechanism of organic reactions by recalling and correlating the fundamental properties of the reactants involved.
- Learn and identify many organic reactions and their mechanisms including electrophilic addition, nucleophilic addition, nucleophilic substitution, electrophilic substitution and rearrangement reactions.

#### SYLLABUS OF DSC-1

##### UNIT – I Fundamentals of organic chemistry (6 Hours)

Types of Electronic displacements: Inductive effect, Resonance effect, Hyperconjugation, Electromeric Effect. Reactive intermediates and their stability: carbocations, free radicals, carbanions, benzyne, carbenes.

Acidity and basicity in organic compounds (comparison of carboxylic acids, alcohols, phenols, primary, secondary and tertiary aliphatic amines, aniline and its derivatives)

## **UNIT – II Stereochemistry (6 Hours)**

Types of projection formulae: Flying Wedge Formula, Newmann, Sawhorse and Fischer representations and their interconversion.

Stereoisomerism: Concept of chirality (upto two carbon atoms). Configurational isomerism: 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).

Conformational isomerism with respect to ethane, butane and cyclohexane.

## **UNIT – III Types of Organic Reactions (Including reactions of alkenes, alkyl and aryl halides, alcohols, aldehydes, ketones) (18 Hours)**

### ***Electrophilic addition reactions***

Electrophilic addition reaction (with respect to propene, propyne, 3,3-dimethyl-1-butene): Hydration, Addition of HX in the absence and presence of peroxide, Hydroboration oxidation, Addition of bromine (with stereochemistry).

### ***Nucleophilic addition reactions***

Nucleophilic addition reaction of carbonyl compounds: Addition of HCN, ammonia derivatives (Hydroxylamine, Hydrazine, Semicarbazide and 2,4-DNP), the addition of carbanion (Aldol condensation, Claisen Schmidt, Benzoin condensation, Perkin reaction, reactions involving Grignard reagent).

### ***Elimination and Nucleophilic substitution reactions***

Nucleophilic substitution reaction ( $S_N1$  and  $S_N2$ ) in alkyl halides (mechanisms with stereochemical aspect), alcohols (with nucleophiles like ammonia, halides, thiols, ambident nucleophiles (cyanide and nitrite ion)), ethers (Williamson ether synthesis), Elimination reaction ( $E1$  &  $E2$ ), elimination *vs* substitution (*w.r.t.* potassium *t*-butoxide and KOH); Nucleophilic aromatic substitution in aryl halides-elimination addition reaction *w.r.t.* chlorobenzene, including the effect of nitro group (on the ring) on the reaction. relative reactivity and strength of C-X bond in alkyl, allyl, benzyl, vinyl and aryl halides towards substitution reactions

### ***Electrophilic substitution reactions***

Electrophilic Aromatic substitution with mechanism (benzene)- sulphonation, nitration, halogenation, Friedel craft acylation :*o*-, *m*- and *p*- directive influence giving examples of toluene/nitrobenzene/ phenol/ aniline/ chlorobenzene.

### ***Reactive intermediates and Rearrangement Reactions***

*Free radicals* (Birch Reduction); *Carbocations* (Pinacol-Pinacolone, Wagner-Meerwein, Rearrangement, and Beckmann rearrangement); *Carbanions* (Michael Addition); *Carbenes* (Reimer-Tiemann).

## **Practical component (60 Hours)**

1. Purification of an organic compound by crystallization (from water and alcohol) and distillation, Criteria of purity: Determination of M.P.
2. Determination of boiling point of liquid compounds. (Boiling point lower than and more than 100 °C by distillation and capillary method)
3. Detection of extra element
4. Preparations: (Mechanism of various reactions involved to be discussed).
  - a. Bromination of phenol/aniline.
  - b. 2,4-Dinitrophenylhydrazone of aldehydes and ketones
  - c. Semicarbazone of aldehydes/ ketones
  - d. Aldol condensation reaction using green method.
  - e. Bromination of Stilbene.
  - f. Acetanilide to p-Bromoacetanilide.

The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization and melting point.

### Essential/recommended readings

#### Theory:

1. Sykes, P.(2003), **A Guide Book to Mechanism in Organic Chemistry**, 6<sup>th</sup> Edition Pearson Education.
2. Eliel, E. L. (2001), **Stereochemistry of Carbon Compounds**, Tata McGraw Hill.
3. Morrison, R. N.; Boyd, R. N., Bhattacharjee, S.K. (2010), **Organic Chemistry**, 7<sup>th</sup> Edition, Pearson Education.

#### Practical:

1. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. (2012), **Vogel's Textbook of Practical Organic Chemistry**, Pearson.
2. Mann, F.G.; Saunders, B.C. (2009), **Practical Organic Chemistry**, Pearson Education.
3. Dhingra, S; Ahluwalia V.K., (2017), **Advanced Experimental Organic Chemistry**, Manakin Press.

### Suggestive readings

#### Theory:

1. Bahl, A; Bahl, B. S. (2019), **Advanced Organic Chemistry**, 22<sup>nd</sup> Edition, S. Chand.

#### Practical:

1. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.

**Note: Examination scheme and modes shall be as prescribed by the Examination Branch, University of Delhi, from time to time.**

## Category II

### BSc. Physical Science with Chemistry as one of the Core Disciplines

#### DISCIPLINE SPECIFIC CORE COURSE – 4:

#### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Periodic Properties and Chemical Bonding DSC-4 Chemistry-II	4	2	0	2	Class Pass 12 <sup>th</sup>	----

#### Learning Objectives

The Learning Objectives of this course are as follows:

- The course discusses the periodicity in properties with reference to the s, p and d block, which is necessary in understanding their group chemistry.
- It provides basic knowledge about ionic, covalent and metallic bonding underlining the fact that chemical bonding is best regarded as a continuum between the three cases.
- It provides an overview of hydrogen bonding and van der Waal's forces which influence the melting points, boiling points, solubility and energetics of dissolution of compounds

#### Learning outcomes

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

- Understand periodicity in ionization enthalpy, electron gain enthalpy, electronegativity and enthalpy of atomization.
- Understand variability in oxidation state, colour, metallic character, magnetic and catalytic properties and ability to form complexes
- Understand the concept of lattice energy using Born-Landé expression.
- Draw Born Haber Cycle and analyse reaction energies.
- Draw the plausible structures and geometries of molecules using VSEPR theory.
- Understand and draw MO diagrams (homo- & hetero-nuclear diatomic molecules). Understand the importance and applications of hydrogen and van der Waal bonding

## SYLLABUS OF DSC-4

### Unit I: Periodic Properties

(12 Hours)

Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy, inert pair effect.

General group trends of s, p and d block elements with special reference to Ionization Enthalpy, Electron Gain Enthalpy, Electronegativity, Enthalpy of Atomization, oxidation state, colour, metallic character, magnetic and catalytic properties, ability to form complexes

### UNIT II: Chemical Bonding

(18 Hours)

**Ionic Bonding:** General characteristics of ionic bonding, Lattice Enthalpy and Solvation Enthalpy and their relation to stability and solubility of ionic compounds, Born-Landé equation for calculation of Lattice Enthalpy (no derivation), Born-Haber cycle and its applications, polarizing power and polarizability, Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

**Covalent Bonding:** Valence Bond Approach, Hybridization and VSEPR Theory with suitable examples, Concept of resonance and resonating structures in various inorganic and organic compounds, Molecular Orbital Approach: Rules for the LCAO method, bonding, nonbonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, MO treatment of homonuclear diatomic molecules of 1<sup>st</sup> and 2<sup>nd</sup> periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO, NO and NO<sup>+</sup>.

Brief introduction to Metallic Bonding, Hydrogen Bonding, van der Waal's Forces

### PRACTICALS:

60 Hours

1. Preparation of standard solutions.
2. Estimation of Sodium carbonate with HCl
3. Estimation of oxalic acid by titrating it with KMnO<sub>4</sub>.
4. Estimation of Mohr's salt by titrating it with KMnO<sub>4</sub>.
5. Estimation of water of crystallization in Mohr's salt by titrating with KMnO<sub>4</sub>.
6. Estimation of Fe (II) ions by titrating it with K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> using internal and external indicators.
7. Estimation of Cu (II) ions iodometrically using Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>.
8. Chromatographic separation of mixture of metal ions Cu<sup>2+</sup>, Cd<sup>2+</sup> or Ni<sup>2+</sup>, Co<sup>2+</sup>.
9. Estimation of Fe (II) ions by titrating it with K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> using
  - a). internal indicator
  - b). external indicator
10. Estimation of Cu (II) ions iodometrically using Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>.
11. Paper Chromatographic separation of mixture of metal ions
  - a). Cu<sup>2+</sup>, Cd<sup>2+</sup>
  - b). Ni<sup>2+</sup>, Co<sup>2+</sup>
12. Any suitable experiment (other than the listed ones) based upon neutralisation/redox reactions.

### References:

### Theory:

1. Huheey, J.E.; Keiter, E.A., Keiter; R. L.; Medhi, O.K. (2009), **Inorganic Chemistry- Principles of Structure and Reactivity**, Pearson Education
2. Shriver, D.D.; Atkins, P.; Langford, C.H. (1994), **Inorganic Chemistry** 2nd Ed., Oxford University Press.
3. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), **Inorganic Chemistry**, 5th Edition, W. H. Freeman and Company.
4. Lee, J.D.; (2010), **Concise Inorganic Chemistry**, Wiley India
5. Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994), **Concepts and Models of Inorganic Chemistry**, John Wiley & Sons.
6. Wulfsberg, G (2002), **Inorganic Chemistry**, Viva Books Private Limited.
7. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), **Inorganic Chemistry**, 5th Edition, Pearson.

**Practical:**

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

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# Bachelor of Sciences (Physical Sciences)

## Category II

**BSc (Physical Sciences) with Chemistry as one of the Core Discipline**

### DISCIPLINE SPECIFIC CORE COURSE -7: Chemistry -III Chemical Energetics and Equilibria

**Credit distribution, Eligibility and Pre-requisites of the Course**

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Chemical Energetics and Equilibria (DSC-7: Chemistry 03:	04	02	0	02	Passed Class 12 <sup>th</sup> with Physics, Chemistry, Mathematics	NIL

### Learning objectives

**The objectives of this course are as follows:**

- To develop basic understanding of the chemical energetics, laws of thermodynamics and ionic equilibrium.
- to provides basic understanding of the behaviour of electrolytes and their solutions.
- To make students learn about the properties of ideal and real gases and deviation from ideal behavior

### Learning outcomes

**By studying this course, students will be able to:**

- Explain the laws of thermodynamics, thermochemistry and equilibria.
- Use the concept of pH and its effect on the various physical and chemical properties of the compounds.
- Use the concepts learnt to predict feasibility of chemical reactions and to study the behaviour of reactions in equilibrium

## SYLLABUS

**UNIT-1: Chemical Energetics**

**(16 Hours)**

Recapitulation of Intensive and extensive variables; state and path functions; Isolated, closed and open systems

### ***First law***

Concept of heat (Q), work (W), internal energy (U), and statement of first law; enthalpy (H), relation between heat capacities for ideal gas, Joule's experiment, calculations of Q, W,  $\Delta U$  and  $\Delta H$  for reversible expansion of ideal gases under isothermal conditions.

### ***Thermochemistry***

Enthalpy of reactions: standard states; enthalpy of neutralization, enthalpy of ionization enthalpy of hydration, enthalpy of formation and enthalpy of combustion, Integral enthalpy of solution, bond dissociation energy and bond enthalpy; Hess's law, Born Haber's cycle (NaCl/KCl).

### ***Second Law***

Concept of entropy; statements of the second law of thermodynamics (Kelvin and Clausius). Calculation of entropy change for reversible processes (for ideal gases). Free Energy Functions: Gibbs and Helmholtz energy (Non-PV work and the work function); Free energy change and concept of spontaneity (for ideal gases).

### ***Third Law***

Statement of third law, qualitative treatment of absolute entropy of molecules (examples of NO, CO), concept of residual entropy

## **UNIT-2: Chemical Equilibrium**

**(4 Hours)**

Criteria of thermodynamic equilibrium. Free energy change in a chemical reaction and equilibrium constant, exergenic and endergenic reactions with examples such conversion of ATP to ADP or vice versa, Le Chatelier's principle, relationship between  $K_p$ ,  $K_c$  and  $K_x$  for reactions involving ideal gases.

## **UNIT-3: Ionic Equilibria**

**(10 Hours)**

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

## **Practical Component:**

**60 Hours**

**(Laboratory periods: 15 classes of 4 hours each)**

### **Chemical Energetics:**

1. Determination of heat capacity of calorimeter.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of the enthalpy of ionization of acetic acid.



4. Determination of enthalpy of neutralization of acetic acid and ammonium hydroxide using Hess's law.
5. Determination of integral enthalpy of solution (both endothermic and exothermic) of salts.
6. Determination of enthalpy of hydration of Copper sulphate.

#### **Ionic equilibria:**

7. Preparation of buffer solutions: (i) Sodium acetate-acetic acid or (ii) Ammonium chloride-ammonium acetate. Measurement of the pH of buffer solutions and comparison of the values with theoretical values.
8. Study the effect of addition of HCl/NaOH on pH of the buffer solutions (acetic acid, and sodium acetate).
9. pH metric titration of strong acid with strong base,
10. pH metric titration of weak acid with strong base

#### **References:**

##### **Theory:**

1. Castellan, G. W. (2004), **Physical Chemistry**, Narosa.
2. Kapoor, K. L. (2015), **A Textbook of Physical Chemistry**, Vol 1, 6<sup>th</sup> Edition, McGraw Hill Education.
3. Kapoor, K. L. (2015), **A Textbook of Physical Chemistry**, Vol 2, 6<sup>th</sup> Edition, McGraw Hill Education.
4. Puri, B. R., Sharma, L. R. and Pathania M. S. (2020), **Principles of Physical Chemistry**, Vishal Publishing Co.

##### **Practical:**

1. Khosla, B. D.; Garg, V. C.; Gulati, A. (2015), **Senior Practical Physical Chemistry**, R. Chand & Co.
2. Kapoor, K. L. (2019), **A Textbook of Physical Chemistry**, Vol 7, 1<sup>st</sup> Edition, McGraw Hill Education.
3. Batra, S. K., Kapoor, V and Gulati, S. (2017) 1<sup>st</sup> Edition, **Experiments in Physical Chemistry**, Book Age series.

#### **Additional Resources:**

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

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## Pool of DISCIPLINE SPECIFIC ELECTIVES (DSEs) for BSC (Physical Science)

### DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -1:

#### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE-1: Main Group Chemistry</b>	<b>04</b>	<b>02</b>	<b>0</b>	<b>02</b>	<b>Passed Class XII with Science</b>	<b>NIL</b>

#### Learning Objectives

The Learning Objectives of this course are as follows:

- To provide basic understanding of the fundamental principles of metallurgy through study of the different methods of extraction and refining of metals.
- To illustrate the diversity and fascination of inorganic chemistry through the study of structure, properties and utilities of s- and p-block elements and their compounds.

#### Learning outcomes

By studying this course, students will be able to:

- Understand the basis of occurrence of metals in nature and the methods that can be applied on minerals to extract the metals from them.
- Explain the importance of free energy of formation of oxides with the choice of reducing agent for extracting the metals.
- Understand and explain the importance of refining of metals and the choice of a refining procedure
- Explain the group trends observed for different properties of s and p block elements
- Explain the structures and the bonding basis of compounds of s- and p- block elements
- Explain the uniqueness observed in alkali metals and some other main group elements
- Understand and explain the polymerization of inorganic ions to generate inorganic polymers and the difference between organic and inorganic polymers.

## Syllabus

### Unit 1: General Principles of Metallurgy

(6 Hours)

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy with reference to cyanide process for silver and gold. Methods of purification of metals: Electrolytic process, Van Arkel-De Boer process, Zone refining.

### Unit 2: General Properties

(4 Hours)

General group trends of s- and p-block elements with special reference to melting and boiling points, flame colour, metallic character and complex formation tendency, diagonal relationship and anomalous behaviour of first member of each group, Alkali metal solutions in liquid ammonia

### Unit 3: Structure, Bonding, Properties and Applications

(16 Hours)

Structure, bonding, properties (Acidic/Basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, thermal stability) and applications of the following:

Crown Ethers and cryptates of Alkali metals

Hydrides: hydrides of Group 13 (only diborane), Group 14, Group 15 ( $\text{EH}_3$  where E = N, P, As, Sb, Bi), Group 16 and Group 17.

Oxides: Oxides of nitrogen, phosphorus and sulphur.

Oxoacids: oxoacids of phosphorus, sulphur and chlorine

Halides of phosphorus

### Unit 4: Inorganic Polymers

(4 Hours)

Preparation, properties, structure and uses of the following:

Borazine, Silicates and Silicones

### Practicals

(60 Hours)

#### (Laboratory periods:60)

Qualitative semi-micro analysis of mixtures containing 2 anions and 2 cations (preferably 7-8 mixtures). Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

$\text{CO}_3^{2-}$ ,  $\text{NO}_2^-$ ,  $\text{S}^{2-}$ ,  $\text{SO}_3^{2-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{S}_2\text{O}_3^{2-}$ ,  $\text{CH}_3\text{COO}^-$ ,  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{NO}_3^-$ ,  $\text{BO}_3^{3-}$ ,  $\text{C}_2\text{O}_4^{2-}$ ,  $\text{PO}_4^{3-}$ ,

$\text{NH}_4^+$ ,  $\text{K}^+$ ,  $\text{Pb}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Bi}^{3+}$ ,  $\text{Sn}^{2+}$ ,  $\text{Sb}^{3+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$

The mixtures may contain combination of anions/one interfering anion.

Spot tests should be preferred wherever applicable.

### **References:**

#### **Theory:**

1. Lee, J.D.; (2010), Concise Inorganic Chemistry, Wiley India.
2. Huheey, J.E.; Keiter, E.A.; Keiter; R. L.; Medhi, O.K. (2009), Inorganic Chemistry- Principles of Structure and Reactivity, Pearson Education.
3. Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994), Concepts and Models of Inorganic Chemistry, John Wiley & Sons.
4. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), Shriver and Atkins Inorganic Chemistry, 5th Edition, Oxford University Press.
5. Housecraft, E. H.; Sharpe, A.G. (2018), Inorganic Chemistry, 5<sup>th</sup> Edition, Pearson.
6. F.A. Cotton & G. Wilkinson (1999), Advanced Inorganic Chemistry, 6<sup>th</sup> Edition, John Wiley & Sons.

#### **Practicals:**

1. Vogel, A.I. (1972), Qualitative Inorganic Analysis, Longman.
2. Svehla, G. (1996), Vogel's Qualitative Inorganic Analysis, Prentice Hall.

**Note:** Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.

## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -2:

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE-2: Polynuclear Hydrocarbons, Pharmaceutical Compounds, UV- Visible &amp; IR Spectroscopy</b>	<b>04</b>	<b>02</b>	<b>0</b>	<b>02</b>	Passed Class XII with Science	<b>NIL</b>

### Learning Objectives

The Learning Objectives of this course are as follows:

- To introduce the chemistry and applications of polynuclear hydrocarbons and heterocyclic compounds.
- Introduction to spectroscopy, an important analytical tool which allows identification of organic compounds by correlating their spectra to structure.

### Learning outcomes

**By studying this course, students will be able to:**

- Understand the fundamentals of polynuclear hydrocarbons and heterocyclic compounds through the study of methods of preparation, properties and chemical reactions with underlying mechanism.
- Gain insight into the basic fundamental principles of IR and UV-Vis spectroscopic techniques.
- Use basic theoretical principles underlying UV-visible and IR spectroscopy as a tool for functional group identification in organic molecules.

## SYLLABUS OF CHEM-DSE-2

### UNIT-1: Polynuclear Hydrocarbons

(6 Hours)

Introduction, classification, uses, aromaticity of polynuclear compounds, Structure elucidation of naphthalene, preparation and properties of naphthalene and anthracene.

## **UNIT-2: Pharmaceutical Compounds**

**(12 Hours)**

Introduction, classification, general mode of action of antipyretics and analgesics, aspirin; Synthesis, uses and side effects of the following drugs:

Antipyretics - Paracetamol (with synthesis and mode of action); Analgesics- Ibuprofen (with synthesis and overview of the mode of action); Antimalarials - Chloroquine (synthesis and mode of action).

An elementary treatment of Antibiotics and detailed study of chloramphenicol including mode of action. Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

## **UNIT-3: UV-Visible and IR Spectroscopy**

**(12 Hours)**

UV-Visible and IR Spectroscopy and their application to simple organic molecules. Electromagnetic radiations and their properties; double bond equivalence and hydrogen deficiency. UV-Visible spectroscopy (electronic spectroscopy): General electronic transitions,  $\lambda_{\max}$  &  $\epsilon_{\max}$ , chromophores & auxochromes, bathochromic & hypsochromic shifts. Application of Woodward rules for the calculation of  $\lambda_{\max}$  for the following systems: conjugated dienes - alicyclic, homoannular and heteroannular;  $\alpha$ ,  $\beta$ -unsaturated aldehydes and ketones, charge transfer complex.

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

## **Practical component**

**60 Hours**

**(Laboratory periods: 15 classes of 4 hours each)**

1. Isolation and estimation of the amount of aspirin in a commercial tablet.
2. Preparation of Aspirin.
3. Synthesis of ibuprofen.
4. Systematic qualitative identification and derivative preparation of organic compounds (Aromatic hydrocarbons, Aryl halides)
5. Detection of simple functional groups through examination of IR spectra (spectra to be provided). IR spectra of simple compounds like phenols, aldehydes, ketones, carboxylic acids may be given.
6. Differentiation between of o-/p-hydroxybenzaldehyde by IR spectroscopy (Spectra to be provided).
7. Differentiation between benzoic acid and cinnamic acid by UV spectroscopy.
8. Diel's Alder reaction using Anthracene and Maleic anhydride.
9. Partial Reduction of m-dinitrobenzene to m-nitroaniline and then analysing the IR spectra of reactant and Product.
10. Laboratory preparation of Paraacetamol.

## **References:**

### **Theory:**

1. Finar, I. L. **Organic Chemistry** (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd.

- (Pearson Education).
2. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
  3. Bahl, A; Bahl, B. S. (2012), **Advanced Organic Chemistry**, S. Chand.
  4. Pavia, D.L. **Introduction to Spectroscopy**, Cengage learning (India) Pvt. Ltd.
  3. Kemp, W. (1991), **Organic Spectroscopy**, Palgrave Macmillan.

#### **Practicals:**

1. Ahluwalia, V.K.; Dhingra, S.; Gulati, A. (2005), **College Practical Chemistry**, University Press (India) Ltd.
2. Ahluwalia, V.K.; Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
3. Vogel, A.I. (1972), **Textbook of Practical Organic Chemistry**, Prentice-Hall.
4. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.
5. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.

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## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE 3:

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE 3: Computer Applications in Chemistry</b>	<b>04</b>	<b>02</b>	<b>0</b>	<b>02</b>	<b>Passed Class XII with Science</b>	<b>NIL</b>

### Learning Objectives

The Learning Objectives of this course are as follows:

- To introduce the students to basic computer skills that will help them in solving chemistry problems using spreadsheets and BASIC language.
- To acquaint the students with different software for data tabulation, calculation, graph plotting, data analysis and document preparation.
- To expose the students to the concept of molecular modelling, its applications to various molecular systems, energy minimization techniques, analysis of Mulliken Charge and ESP Plots.

### Learning outcomes

**By studying this course, students will be able to:**

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

## SYLLABUS OF CHEM-DSE-3

### UNIT-1: Programming using BASIC

**(20 Hours)**

Programming Language – Elements of BASIC language, Numeric and string Constants and Variables, arithmetic expressions, hierarchy of operations, inbuilt functions. Syntax and use of the various QBASIC commands: REM, CLS, INPUT, PRINT, GOTO, IF, IF...THEN, IF..THEN..ELSE, IF and END IF, FOR and NEXT etc., DIM, READ, DATA, GOSUB,



RETURN, RESTORE, DEF FNR and Library Functions, Simple programs based on usage of the commands mentioned above.

Statistical analysis using BASIC: Mean, Least square fit - Linear regression, variance, standard deviation.

## **UNIT-2: Handling of Numerical Data (4 Hours)**

Spreadsheet software: MS Excel. Creating a spreadsheet, entering and formatting information, applying basic functions and formulae to the data, drawing charts, tables and graphs, displaying the equation of graph along with the  $R^2$  value, incorporating tables and graphs in Word files, graphical solution of equations, plotting pressure-volume curves of van der Waals gases, Maxwell-Boltzmann distribution, concentration versus time graphs, spectral data, titration curves, etc.

## **UNIT-3: Molecular Modelling (6 Hours)**

Introduction to molecular modelling, overview of classical and quantum mechanical methods (molecular mechanics, semi empirical, ab initio and DFT), general considerations and comparison of these methods.

## **Practical component (Laboratory periods: 15 classes of 4 hours each) 60 Hours**

### **Exercises of Programing**

1. Calculate pressure of a real gas using Van der Waal's Equation.
2. Calculate the most probable speed, average speed and root mean square velocity of an ideal gas.
3. Roots of quadratic equations
4. Binomial coefficient using GOSUB statement.
5. Mean, standard deviation
6. Least square curve fitting method for linear equation.

### **Plotting graphs using a spreadsheet**

1. van der Waals isotherms
2. Maxwell-Boltzmann distribution curves as function of temperature and molecular weight
3. Plot the conductometric titration curve for
  - a) strong acid vs strong base and b) weak acid vs strong base
4. Plot the pH metric titration curve for
  - a) strong acid vs strong base and b) weak acid vs strong base and determine the  $pK_a$  of the weak acid
5. Plot the graphs for the kinetics of first order reaction and determine the rate constant
6. Plot the UV-vis absorbance spectra and determine the molar absorption coefficient.

### **Molecular Modelling**

1. Optimize and compare the geometry parameters of H<sub>2</sub>O and H<sub>2</sub>S using Argus Lab.
2. Compare the basicities of N atom in ammonia, methylamine, dimethylamine and trimethylamine using Argus Lab by comparing Mulliken charges and ESP map in Argus Lab.
3. Compare C-C bond lengths and bond order in ethane, ethene and ethyne using Argus Lab.
4. Determine enthalpy of isomerization of cis and trans-2-butene in Argus Lab.
5. Compare the HAH bond angles for the second row hydrides (BeH<sub>2</sub>, CH<sub>4</sub>, NH<sub>3</sub>, H<sub>2</sub>O) and compare with the results from qualitative MO theory.

### References:

#### Theory:

1. Levie, R. de. (2001), **How to use Excel in analytical chemistry and in general scientific data analysis**, Cambridge Univ. Press.
2. Venit, S.M. (1996), **Programming in BASIC: Problem solving with structure and style**. Jaico Publishing House.
3. Lewars, E. (2003), **Computational Chemistry**, Kluwer academic Publisher.
4. Cramer, C.J.(2004), **Essentials of Computational Chemistry**, John Wiley & Sons.
5. Hinchcliffe, A. (1996), **Modelling Molecular Structures**, John Wiley & Sons.
6. Leach, A.R.(2001), **Molecular Modelling**, Prentice-Hall.

#### Practicals:

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

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**BSC. (PHYSICAL SCIENCES)- CHEMISTRY COMPONENT**  
**SEMESTER -VI**

**DISCIPLINE SPECIFIC CORE COURSE -16: Chemistry -VI Quantum Chemistry and Spectroscopy**

**CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE**

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Quantum Chemistry and Spectroscopy DSC-16: Chemistry-VI</b>	<b>04</b>	<b>02</b>	<b>--</b>	<b>02</b>	<b>Class 12th with Physics, Chemistry, Mathematics</b>	<b>NA</b>

**Learning Objectives**

The Learning Objectives of this course are as follows:

- To introduce the concepts and methodology of quantum mechanics
- Application of Quantum chemistry to spectroscopy
- To establish the relation between structure determination and spectra.

**Learning outcomes**

By studying this course, students will be able to:

- Understand basic principles of quantum mechanics: operators, eigen values, averages, probability distributions.
- Understand and use basic concepts of microwave, IR and UV-VIS spectroscopy for interpretation of spectra.

**Syllabus**

**Unit 1: Quantum Chemistry**

**(Hours: 16)**

Postulates of quantum mechanics, quantum mechanical operators.

Schrodinger equation and its application to free particle and particle in a 1-D box (complete solution), quantization, normalization of wave functions, concept of zero-point energy.

Qualitative treatment of H and H like atoms. Setting up of Schrodinger equation for many electron atoms.

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

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

## **Unit 2: Spectroscopy**

**(Hours: 14)**

Electromagnetic radiation and its interaction with matter. Lambert-Beer's law, Jablonski's diagram. Florescence and Phosphorescence.

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

*Microwave Spectroscopy:* Microwave (pure rotational) spectra of diatomic molecules. Selection rules.

Structural information derived from rotational spectroscopy.

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

*Electronic Spectroscopy:* Electronic excited states. Free electron model and its application to electronicspectra of polyenes. chromophores, auxochromes, bathochromic and hypsochromic shifts.

## **Practical component**

**Credits:02**

**(Laboratory periods: 60 )**

### **UV/Visible spectroscopy**

1. 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).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of  $\text{K}_2\text{Cr}_2\text{O}_7$
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of

organic compounds.

### Colorimetry

4. Verify Lambert-Beer's law and determine the concentration of  $\text{CuSO}_4$ /  $\text{KMnO}_4$ /  $\text{K}_2\text{Cr}_2\text{O}_7$ /  $\text{CoCl}_2$  in a solution of unknown concentration
5. Determine the concentrations of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  in a mixture.
6. Study the kinetics of iodination of propanone in acidic medium.
7. Determine the amount of iron present in a sample using 1, 10-phenanthroline.
8. Determine the dissociation constant of an indicator (phenolphthalein).
9. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

### References:

#### Theory:

1. Banwell, C.N.; McCash, E.M.(2006), **Fundamentals of Molecular Spectroscopy**, Tata McGraw- Hill.
2. Kapoor, K.L.(2015), **A Textbook of Physical Chemistry**, McGraw Hill Education, Vol 4, 5<sup>th</sup> Edition, McGraw Hill Education.
3. McQuarrie, D.A.(2016), **Quantum Chemistry**, Viva Books.
4. Chandra, A. K.(2001), **Introductory Quantum Chemistry**, Tata McGraw-Hill.
5. Dua A and Tyagi P, **Molecular Spectroscopy: Quantum to Spectrum**, (2022) Atlantic Publishers & Distributors Pvt Ltd.
6. Dua A, Singh C, **Quantum Chemistry: Classical to Computational** (2015) ManakinPress.

#### Practical:

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), **Senior Practical Physical Chemistry**, R. Chand & Co, New Delhi.
2. Kapoor, K.L. (2019), **A Textbook of Physical Chemistry**, Vol.7, 1<sup>st</sup> Edition, McGraw Hill Education.
3. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P.( 2003), **Experiments in Physical Chemistry**, 8<sup>th</sup> Edition, McGraw-Hill, New York.

#### Additional Resources:

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

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## POOL OF DISCIPLINE SPECIFIC ELECTIVES FOR SEMESTER -III/IV/V/VI

### SEMESTER III

#### DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -1: Main Group Chemistry

#### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical / Practice		
<b>Chem-DSE 1: Main Group Chemistry</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

#### Learning Objectives

The Learning Objectives of this course are as follows:

- To provide basic understanding of the fundamental principles of metallurgy through study of the different methods of extraction and refining of metals.
- To illustrate the diversity and fascinating aspects of inorganic chemistry through the study of structure, properties and utilities of s- and p-block elements and their compounds.

#### Learning outcomes

By studying this course, students will be able to:

- Understand the basis of occurrence of metals in nature and the methods that can be applied on minerals to extract the metals from them.
- Explain the importance of free energy of formation of oxides with the choice of reducing agents for extracting the metals.
- Understand and explain the importance of refining of metals and the choice of a refining procedure.
- Explain the group trends observed for different properties of s and p block elements.
- Explain the structures and the bonding of compounds of s- and p- block elements
- Explain the unique properties of alkali metals and some other main group elements
- Understand and explain the polymerization mechanism of inorganic ions to generate inorganic polymers and the difference between organic and inorganic polymers.

#### Syllabus

## Unit 1: General Principles of Metallurgy

(Hours: 6)

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy with reference to cyanide process for silver and gold. Methods of purification of metals: Electrolytic process, Van Arkel-De Boer process, Zone refining.

## Unit 2: General Properties

(4 Hours)

General group trends of s- and p-block elements with special reference to melting and boiling points, flame colour, metallic character and complex formation tendency, diagonal relationship and anomalous behaviour of first member of each group, Alkali metal solutions in liquid ammonia

## Unit 3: Structure, Bonding, Properties and Applications

(Hours: 16)

Structure, bonding, properties (Acidic/Basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, thermal stability) and applications of the following:

Crown Ethers and cryptates of Alkali metals

Hydrides: hydrides of Group 13 (only diborane), Group 14, Group 15 ( $\text{EH}_3$  where E = N, P, As, Sb, Bi), Group 16 and Group 17.

Oxides: Oxides of nitrogen, phosphorus and sulphur.

Oxoacids: oxoacids of phosphorus, sulphur and chlorine

Halides of phosphorus

## Unit 4: Inorganic Polymers

(4 Hours)

Preparation, properties, structure and uses of the following:  
Borazine, Silicates and Silicones.

## Practicals

Credits:02

### (Laboratory periods:60)

Qualitative semi-micro analysis of mixtures containing 2 anions and 2 cations (preferably 7-8 mixtures). Emphasis should be given to the understanding of the chemistry of different reactions.

The following radicals are suggested:

$\text{CO}_3^{2-}$ ,  $\text{NO}_2^-$ ,  $\text{S}^{2-}$ ,  $\text{SO}_3^{2-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{S}_2\text{O}_3^{2-}$ ,  $\text{CH}_3\text{COO}^-$ ,  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{NO}_3^-$ ,  $\text{BO}_3^{3-}$ ,  $\text{C}_2\text{O}_4^{2-}$ ,  $\text{PO}_4^{3-}$ ,  $\text{NH}_4^+$ ,  $\text{K}^+$ ,  $\text{Pb}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Bi}^{3+}$ ,  $\text{Sn}^{2+}$ ,  $\text{Sb}^{3+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ .

The mixtures may contain combination of anions/one interfering anion.

Spot tests should be preferred wherever applicable.

## References:

## Theory:

1. Lee, J.D.; (2010), **Concise Inorganic Chemistry**, Wiley India.
2. Huheey, J.E.; Keiter, E.A.; Keiter; R. L.; Medhi, O.K. (2009), **Inorganic Chemistry- Principles of Structure and Reactivity**, Pearson Education.
3. Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994), **Concepts and Models of Inorganic Chemistry**, John Wiley & Sons.
4. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), **Shriver and Atkins Inorganic Chemistry**, 5th Edition, Oxford University Press.
5. Housecraft, E. H.; Sharpe, A.G. (2018), **Inorganic Chemistry**, 5<sup>th</sup> Edition, Pearson.
6. F.A. Cotton & G. Wilkinson (1999), **Advanced Inorganic Chemistry**, 6<sup>th</sup> Edition, John Wiley & Sons.

#### **Practicals:**

1. Vogel, A.I. (1972), **Qualitative Inorganic Analysis**, Longman.
2. Svehla, G. (1996), **Vogel's Qualitative Inorganic Analysis**, Prentice Hall.
3. Dua A, Manav N, **Practical Inorganic Chemistry**, (2017), Manakin Press.

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## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -2: Green Chemistry

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE-2: Green Chemistry</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

The Learning Objectives of this course are as follows:

- To learn about the environmental status, public awareness in evolution, principles involved in green chemistry, bio-catalytic reactions, global warming and its control measures, availability of green analytical methods.
- To practice chemistry in the safest way possible
- To imbibe safeworking conditions in the laboratories as well as the chemical industry extending to society in a sustainable future for the planet.

### Learning outcomes

By studying this course, students will be able to:

- Understand the twelve principles of green chemistry and also build the basic understanding of toxicity, hazard and risk related to chemical substances.
- Calculate atom economy, E-factor and relate them in all organic synthesis
- Appreciate the use of catalyst over stoichiometric reagents
- Learn to use green solvents, renewable feedstock and renewable energy sources for carrying out safer chemistry
- Appreciate the use of green chemistry in problem solving skills and critical thinking to innovate and find solutions to environmental problems.
- Learn to design safer processes, chemicals and products through understanding of inherently safer design (ISD)
- Appreciate the success stories and real-world cases as motivation for them to practice green chemistry

### Syllabus

## **Unit 1: Introduction**

**(Hours: 8)**

Definition of green chemistry and how it is different from conventional chemistry and environmental chemistry.

Need of green chemistry.

Importance of green chemistry in- daily life, Industries and solving human health problems (four examples each).

A brief study of Green Chemistry Challenge Awards (Introduction, award categories and study about five last recent awards).

## **Unit 2: Twelve Principles of Green Chemistry**

**(Hours: 12)**

The twelve principles of the Green Chemistry with their explanations Special emphasis on the following:

- Prevention of waste / by products, pollution prevention hierarchy.
- Green metrics to assess greenness of a reaction: environmental impact factor, atom economy and calculation of atom economy.
- Green solvents-supercritical fluids, water as a solvent for organic reactions, ionic liquids, solvent less reactions, solvents obtained from renewable sources.
- Catalysis and green chemistry- comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
- Green energy and sustainability.
- Real-time analysis for pollution prevention.

Prevention of chemical accidents, designing greener processes, principles of inherent safer design (ISD). Bhopal Gas Tragedy (safer route to carbaryl) and Flixborough accident (safer route to cyclohexanol), subdivision of ISD, minimization, simplification, substitution, moderation and limitation.

## **Unit 3: Real-world Cases in Green Chemistry**

**(Hours: 10)**

Discussion of the following Real-world Cases in green chemistry: 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. Right fit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments. An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn.

## **Practical Component**

**Credits:02**

**(Laboratory periods:60)**

Characterization by melting point, UV-Visible spectroscopy, IR spectroscopy and any other specific method should be done (wherever applicable).

1. Preparation and characterization of nanoparticles of gold using tea leaves/silver nanoparticles using plant extracts.
2. Preparation of biodiesel from waste cooking oil and characterization (TLC, pH, solubility, combustion test, density, viscosity, gel formation at low temperature and IR can be provided).
3. Benzoin condensation using thiamine hydrochloride as a catalyst instead of cyanide.
4. Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice.
5. Mechanochemical solvent free, solid-solid synthesis of azomethine using p-toluidine and o-vanillin/p-vanillin.
- 6 Microwave-assisted Knoevenagel reaction using anisaldehyde, ethyl cyanoacetate and ammonium formate.
7. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
8. Photochemical conversion of dimethyl maleate to dimethyl fumarate (cis-trans isomerisation)
9. Benzil- Benzilic acid rearrangement: Preparation of benzilic acid in solid state under solvent-free condition.

**References:****Theory:**

1. Anastas, P.T., Warner, J.C. (2014), **Green Chemistry, Theory and Practice**, Oxford University Press.
2. Lancaster, M. (2016), **Green Chemistry: An Introductory Text**, 3rd Edition, RSC Publishing.
3. Cann, M. C., Connely, M.E. (2000), **Real-World cases in Green Chemistry**, American Chemical Society, Washington.
4. Matlack, A.S. (2010), **Introduction to Green Chemistry**, 2nd Edition, Boca Raton: CRC Press/Taylor & Francis Group publisher.
5. Alhuwalia, V.K., Kidwai, M.R. (2005), **New Trends in Green chemistry**, Anamalaya Publishers.
6. Sidhwani, I.T, Sharma, R.K. (2020), **An Introductory Text on Green Chemistry**, Wiley India Pvt Ltd.

**Practicals:**

7. Kirchoff, M.; Ryan, M.A. (2002), **Greener approaches to undergraduate chemistry experiment**, American Chemical Society, Washington DC.

8. Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K. (2013), **Green Chemistry Experiments: A monograph**, I.K. International Publishing House Pvt Ltd. New Delhi.
9. Pavia, D.L.; Lamponam, G.H.; Kriz, G.S.W. B. (2012), **Introduction to organic Laboratory Technique- A Microscale approach**, 4th Edition, Brooks-Cole Laboratory Series -for Organic chemistry.
10. Sindhwani I.T. (2015), **Wealth from Waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated**. DU Journal of Undergraduate Research and Innovation, 1(1),131-151. ISSN: 2395- 2334.
11. Sidhwani, I.T; Sharma, R.K. (2020), **An Introductory Text on Green Chemistry**, Wiley India Pvt Ltd.
12. **Monograph on Green Chemistry Laboratory Experiments**, Green Chemistry Task Force Committee, Department of Science and Technology, Government of India.

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## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE 3: Chemistry of Colloids and Adsorption

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE 3: Chemistry of Colloids and Adsorption</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

**The Learning Objectives of this course are as follows:**

- To develop basic concepts of colloids and colloidal phenomenon.
- Preparation and characterization of sols, understanding about applications of colloid in food, petroleum and cosmetic industry.
- Basic understanding of adsorption, types of adsorption, chemistry of adsorption and its applications.

### Learning outcomes

**By studying this course, students will be able to:**

- Understand colloid solutions, preparation of sols.
- Understand the concept of Electrical double layer, charge on colloidal particles.
- Characterize the colloids sols, learn colloid phenomenon like Tyndall effect, Brownian movement, electrophoresis, dialysis, coagulation and flocculation.
- Understand adsorption, types of adsorption. Characteristics, factors affecting adsorption and its applications

### Syllabus

#### **Unit 1: Colloidal State**

**(Hours: 8)**

Distinction among true solutions, colloids and suspensions, components of Colloids, classification of colloids - lyophilic, lyophobic; Preparation methods and properties of lyophobic solutions, Hydrophile-lyophile balance (HLB), multi molecular, macromolecular and associated colloids (micelles formation), Schulze -Hardy law.

#### **Unit 2: Preparation and Properties of Colloids**

**(Hours: 14)**

Methods of preparation of colloids, Tyndall effect, Brownian movement, coagulation and flocculation; electrophoresis, dialysis.

Emulsification by surfactants, selection of surfactants as emulsifying agent, colloidal phenomenon in food chemistry, Protein based functional colloids.

### **Unit 3: Surface Chemistry**

**(Hours: 8)**

Adsorption, Distinction between adsorption and absorption, Types of Adsorption, Physisorption and chemisorption and their characteristics, factors affecting adsorption of gases on solids - Freundlich and Langmuir adsorption isotherms, Adsorption from solutions. Applications of Adsorption phenomenon in living systems.

### **Practical component**

**Credits: 02**

**(Laboratory periods: 60)**

1. Preparation of Colloidal Sols of following
  - a. Egg Albumin
  - b. Starch /Gum
  - c. Ferric chloride
  - d. Aluminum hydroxide
  - e. Antimony Sulphide
2. To find out the precipitation values of Antimony Sulphide sol by using monovalent, bivalent and trivalent cations.
3. To verify the Schulze -Hardy law.
4. To verify the Freundlich's Adsorption isotherms.
5. Study of adsorption of HAc on charcoal and prove the validity of Langmuir's adsorption isotherms
6. Study of adsorption of Oxalic acid on charcoal and prove the validity of Langmuir's adsorption isotherms.

### **References:**

#### **Theory:**

1. Puri B. R., Sharma L. R. and Pathania M.S., (2020) Principles of Physical Chemistry, Vishal Publishing Co. Jalandhar, Punjab, India.
2. Kapoor K L, **Text Book of Physical Chemistry, Vol. 4**, McGraw Hill Education (India) Private Limited, Chennai, India.
3. Evans D F and Wennerström's, **The Colloidal Domain**, Second Edition, John Wiley & Sons Inc.
4. Adamson A. W. and Gast A., **Physical Chemistry of Surfaces** (Main text) Sixth Edition, John Wiley & Sons Inc.
5. Berg J. C., **An Introduction to Interfaces and Colloids**, World Scientific Publishing Co., Inc. New Jersey.
6. Israelachvili J. N., **Intermolecular and Surface Forces**, Elsevier Inc.

**Practical:**

1. Giri, S; Bajpai, D.N.; Pandey, O.P. **Practical Chemistry**, S. Chand Limited.
2. Khosla, B.D.; Garg, V.C.; Gulati, A.(2015), **Senior Practical Physical Chemistry**, R. Chand & Co.

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## SEMESTER IV

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

#### DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -4: Nanoscale Materials and their Applications

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE-4: Nanoscale Materials and their Applications</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

The Learning Objectives of this course are as follows:

- To introduce nanoscale materials and their applications.
- To provide an insight into bottom-up and top-down-approach, the methods of synthesis of nanoparticles, simple characterization techniques and applications of nanomaterials.

### Learning outcomes

By studying this course, students will be able to:

- Understand the concept of nano dimensions.
- Know the various methods of preparation of nanomaterials.
- Understand the principles of optical and electron microscopy techniques of characterizing nanomaterials.
- Understand and appreciate the real life applications of nanomaterials.

### Syllabus

#### **Unit 1: Introduction to Nanodimensions**

**(Hours: 12)**

0D, 1D, 2D nanomaterials, Quantum Dots, Nanoparticles, Nanostructures (nanowires, thin films, nanorods), carbon nanostructures (carbon nanotubes, carbon nanofibers, fullerenes), Size Effects in nano systems, Quantum confinement and its consequences, Semiconductors. Band structure and band gap. Optical Properties Surface plasmon resonance

#### **Unit 2: Preparation of Nanomaterials**

**(Hours: 10)**



Top down and Bottom up approach, Photolithography. Ball milling. Vacuum deposition. Physical vapor deposition (PVD), Chemical vapor deposition (CVD), Thermal decomposition, Chemical reduction, Sol-Gel synthesis, Hydrothermal synthesis, Spray pyrolysis, Electrochemical deposition, Pulsed Laser deposition. Characterization of nanomaterials: Basic principle of optical methods and electron microscopy.

### **Unit 3: Applications of Nanomaterials**

**(Hours: 8)**

Nanomaterials as Catalysts, semiconductor nanomaterials as photocatalysts, Nanocomposites as catalysts. Carbon nanostructures as catalytic nanoreactors, metal and metal oxides confined inside carbon nanostructures, Nanowires and thin films for photonic devices (LEDs, solar cells, transistors).

### **Practical Component**

**Credits:02**

**(Laboratory periods:60)**

1. Synthesis of silver nanoparticles by chemical methods and characterization using UV-visible spectrophotometer.
  - a. Turkevich Method
  - b. Burst Method
2. Synthesis of silver nanoparticles by green approach methods (using soluble starch, glucose or cinnamon bark) and characterization using UV-visible spectrophotometer.
3. Synthesis of metal sulphide nanoparticles and characterization using UV-visible spectrophotometer.
  - a. MnS
  - b. ZnS
  - c. CuS
4. Intercalation of hydrogen in tungsten trioxide and its conductivity measurement using conductometer.
5. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.
6. Phytochemicals mediated synthesis of gold nanoparticles (AuNPs) using tea leaves and to study the effect of size on color of gold/silver nanoparticles.
7. Preparation of magnetic nanoparticles (MNPs) of Fe<sub>3</sub>O<sub>4</sub> using green tea leaf extract.
8. Any suitable experiment (other than the listed ones) based upon complexation reactions.

### **References:**

#### **Theory:**

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

4. Poole Jr.; Charles P.; Owens, Frank J. (2003), **Introduction to Nanotechnology**, John Wiley and Sons. Inc. Harris, D. C. (2007), **Quantitative Chemical Analysis**, 6th Edition, Freeman.
5. Chattopadhyay, K.K.; Banerjee, A. N. (2009), **Introduction to Nanoscience and Technology**, Prentice Hall India.

**Practicals:**

1. Orbaek, W.; McHale, M.M.; Barron, A. R.; **Synthesis and Characterization of Silver Nanoparticles for An Undergraduate Laboratory**, J. Chem. Educ. 2015, 92, 339–344.
2. MacDiarmid, G.; Chiang, J.C.; Richter, A.F.; Somasiri, N.L.D.(1987), **Polyaniline: Synthesis and Characterization of the Emeraldine Oxidation State by Elemental Analysis**, L. Alcaer (ed.), Conducting Polymers, 105-120, D. Reidel Publishing.

**Note:** Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.

## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -5: Molecules of Life

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE-5: Molecules of Life</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

The Learning Objectives of this course are as follows:

- To deliver information about the chemistry of carbohydrates, proteins & enzymes and its relevance in the biological system using suitable examples.
- To provide an insight into the structural principles that govern reactivity/physical /biological properties of biomolecules as opposed to learning structural details.

### Learning outcomes

By studying this course, students will be able to:

- Learn and demonstrate how the structure of biomolecules determines their chemical properties, reactivity and biological uses.
- Gain an insight into the mechanism of enzyme action and inhibition.
- Understand the basic principles of drug-receptor interaction and SAR.

### Syllabus

#### **Unit 1: Carbohydrates**

**(Hours: 12)**

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

#### **Unit 2: Amino acids, Peptides and Proteins**

**(Hours: 10)**

Classification of amino acids and biological uses of amino Acids, peptides and proteins. Zwitterion structure, isoelectric point and correlation to acidity and basicity of amino acids. Determination of primary structure of peptides, determination of N-terminal amino acid (by Edman method) and C–

terminal amino acid (with carboxypeptidase enzyme). Synthesis of simple peptides (up to dipeptides) by N-protection (t-butyloxycarbonyl) & C-activating groups (only DCC) and Merrifield solid phase synthesis, Overview of primary, secondary, tertiary and quaternary structure of proteins, denaturation of proteins.

### **Unit 3: Enzymes**

**(Hours: 4)**

Classification of enzymes and their uses (mention Ribozymes). Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in enzyme action, specificity of enzyme action (including stereospecificity).

-

### **Unit 4: Nucleosides, Nucleotides and Nucleic Acids**

**(Hours: 4)**

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

### **Practical Component**

**Credits:02**

#### **(Laboratory periods:60)**

1. Estimation of glucose by Fehling's solution.
2. Determination of total sugar content by ferricyanide method (volumetric/colorimetric method).
3. Study of the titration curve of glycine and determine the isoelectric point of glycine.
4. Estimation of proteins by Lowry's method.
5. Qualitative tests for amino acids, proteins and carbohydrates.
6. Separation and identification of mixture of sugars by paper chromatography.
7. Separation and identification of mixture of Amino acids by paper chromatography.
8. Study of the action of salivary amylase on starch under optimum conditions and find the enzyme activity.
9. Study the effect of temperature on activity of salivary amylase.
10. Extraction of DNA from onion/cauliflower.

### **References:**

#### **Theory:**

1. Finar, I. L. **Organic Chemistry (Volume 1 & 2)**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Morrison, R. N.; Boyd, R. N., Bhattacharjee, S.K. (2010), **Organic Chemistry, 7th Edition**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education India).
3. Berg, J. M.; Tymoczko, J. L.; Stryer, L. (2019), **Biochemistry, 9th Ed.**, W. H. Freeman Co Ltd.

**Practicals:**

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

**Note:** Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.

## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -6: Conductance, Electrochemistry and Chemical Kinetics

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE 6: Conductance, Electrochemistry and Chemical Kinetics</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

The Learning Objectives of this course are as follows:

- To develop basic understanding of electrolytic and galvanic cells.
- Measurement of conductance and its applications, measurement of emf and its applications.
- To understand reaction rate, order, activation energy and theories of reaction rates.

### Learning outcomes

By studying this course, students will be able to:

- Explain the factors that affect conductance, migration of ions and application of conductance measurement.
- Understand the importance of Nernst equation, measurement of emf, calculations of thermodynamic properties and other parameters from the emf measurements.
- Understand rate law and rate of reaction, theories of reaction rates and catalysts; both chemical and enzymatic.

### Syllabus

#### Unit 1: Conductance

**(Hours: 8)**

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes, Kohlrausch Law of independent migration of ions, Ionic velocity, mobility and their determination, transference number and its relation to ionic mobility, Conductometric titrations (only acid-base).

## Unit 2: Electrochemistry

(Hours: 12)

Concept of reversible and irreversible electrochemical cells, Standard hydrogen electrode, standard electrode potential, concept of EMF of a cell, measurement of EMF of a cell, Nernst equation and its importance, types of electrodes (Reference and inert electrodes), 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. pH determination using glass electrode, Potentiometric titrations-qualitative treatment (acid-base and oxidation-reduction only).

## Unit 3: Chemical Kinetics and Catalysis

(Hours: 10)

The concept of reaction rates, effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction, integrated rate equations for zero, first and second order reactions (derivation not required), half-life of a reaction, Concept of activation energy and its calculation from Arrhenius equation.

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

## Practical component

Credits:02

### Laboratory periods: 60

1. Determination of molar conductance, degree of dissociation and dissociation constant of a weak acid.
2. Perform the following conductometric titrations: Strong acid vs strong base.
3. Perform the following conductometric titrations: Weak acid vs strong base.
4. Determination of TDS of water from different sources.
5. Determination of Soil pH of soil collected from various locations.
6. Perform the potentiometric titrations of strong acid vs strong base
7. Perform the potentiometric titrations of Weak acid vs strong base.
8. Perform the potentiometric titrations of Potassium dichromate vs. Mohr's salt.
9. Perform the potentiometric titrations of  $\text{KMnO}_4$  vs. Mohr's salt.
10. Study the kinetics of acid hydrolysis of methyl acetate with hydrochloric acid.

## References:

## Theory:

1. Castellan, G. W. (2004), **Physical Chemistry**, Narosa Publications.
2. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol.1, 6<sup>th</sup> Edition, McGraw Hill Education.
3. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol.5, 3<sup>rd</sup> Edition, McGraw Hill Education.
4. Puri, B.R., Sharma, L.R. and Pathania M.S. (2020), **Principles of Physical Chemistry**, Vishal Publishing Co.

\*

#### **Practicals:**

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), **Senior Practical Physical Chemistry**, R. Chand & Co. Kapoor, K.L. (2019), **A Textbook of Physical Chemistry**, Vol 7, 1<sup>st</sup> Edition, McGrawHill Education.
2. Batra, S.K., Kapoor, V and Gulati, S. (2017) 1<sup>st</sup> Edition, **Experiments in Physical Chemistry**, Book Age series.

**Note:** Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.



## SEMESTER V

### DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -7: Inorganic Materials of Industrial Importance

#### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE-7: Inorganic Materials of Industrial Importance</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

#### Learning Objectives

The Learning Objectives of this course are as follows:

- The course introduces learners to the importance of Inorganic compounds in Industries.
- To provide an insight into how the inorganic materials form a basis of the products used in day-to-day life like silicates, fertilizers, surface coatings.

#### Learning outcomes

By studying this course, students will be able to:

- Learn the composition and applications of the different kinds of glass.
- Understand glazing of ceramics and the factors affecting their porosity.
- Give the composition of cement and discuss the mechanism of setting of cement.
- Explain the suitability of fertilizers for different kinds of crops and soil.
- Understand and explain the polymerization of inorganic ions to generate inorganic polymers and the difference between organic and inorganic polymers.

#### Syllabus

##### Unit 1: Silicate Industries

(Hours: 10)

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime

glass, lead glass, armoured glass, different types of safety glass, borosilicate glass, fluorosilicate glass, coloured glass, photosensitive glass, photochromic glass, glass wool and optical fibre.

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

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

## **Unit 2: Fertilizers**

**(Hours: 8)**

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

## **Unit 3: Surface Coatings**

**(Hours: 12)**

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

### **Practical Component**

**Credits:02**

**(Laboratory periods:60)**

1. Detection of constituents of CAN fertilizer (Calcium, Ammonium and Nitrate ions) fertilizer and estimation of Calcium content.
2. Detection of constituents of Superphosphate fertilizer (Calcium and Phosphate ions) and estimation of phosphoric acid content.
3. Detection of constituents of Dolomite (Calcium, Magnesium and carbonate ions) and determination of composition of Dolomite (Complexometric titration).
4. Analysis of (Cu, Ni) in alloy or synthetic samples (Multiple methods involving Complexometry, Gravimetry and Spectrophotometry).
5. Analysis of (Cu, Zn) in alloy or synthetic samples (Multiple methods involving Iodometry, Complexometry and Potentiometry).
6. Preparation of following Inorganic Pigments:
  - a). Barium white
  - b). Chrome Yellow

- c). Malachite
  - d).Chromium oxide
  - e). Prussian Blue
7. Any suitable experiment other than the listed ones.

#### References:

#### Theory:

1. West, A. R. (2014), **Solid State Chemistry and Its Application**, Wiley & sons.
2. Smart, L. E.; Moore, E. A. (2012), **Solid State Chemistry An Introduction**, CRC Press Taylor & Francis.
3. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A.(2010), **Inorganic Chemistry**, W. H. Freeman and Company.
4. Kent, J. A. (ed) (1997), **Riegel's Handbook of Industrial Chemistry**, CBS Publishers, New Delhi.
5. Jain P.C., Jain M., **Engineering Chemistry**, Dhanpat Rai & Sons, Delhi.
6. Gopalan R., Venkappaya D.,Nagarajan S., **Engineering Chemistry**, Vikas Publications, New Delhi.
7. Sharma, B.K., **Engineering Chemistry**, Goel Publishing House, Meerut.
8. Kingery W.D., Bowen H. K., Uhlmann, D.R., (1976), **Introduction to Ceramics**, Wiley & sons, Delhi.

#### Practicals:

1. Vogel A. I., Vogel's **Quantitative Inorganic Analysis**, Pearson Education.
2. Banewicz, J. J.; Kenner, C.T. **Determination of Calcium and Magnesium in Limestones and Dolomites**, Anal. Chem., 1952, 24 (7), 1186–1187.

**Note:** Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.

**DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE 8: Polynuclear Hydrocarbons,  
Pharmaceutical Compounds, UV- Visible & IR Spectroscopy**

**CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE**

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE 8: Polynuclear Hydrocarbons, Pharmaceutical Compounds, UV- Visible &amp; IR Spectroscopy</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

The Learning Objectives of this course are as follows:

- To provide an insight to the fundamentals of polynuclear hydrocarbons and heterocyclic compounds
- The course introduces learners to IR and UV-Vis spectroscopic techniques and their importance in functional group identification.

### Learning outcomes

By studying this course, students will be able to:

- Understand the fundamentals of polynuclear hydrocarbons and heterocyclic compounds through the study of methods of preparation, properties and chemical reactions with underlying mechanism.
- Gain insight into the basic fundamental principles of IR and UV-Vis spectroscopic techniques.
- Use basic theoretical principles underlying UV-visible and IR spectroscopy as a tool for functional group identification in organic molecules.

### Syllabus

#### UNIT-1: Polynuclear Hydrocarbons

**(Hours: 6)**

Introduction, classification, uses, aromaticity of polynuclear compounds, Structure elucidation of naphthalene, preparation and properties of naphthalene and anthracene.

## UNIT-2: Pharmaceutical Compounds

(Hours: 12)

Introduction, classification, general mode of action of antipyretics and analgesics, aspirin; Synthesis, uses and side effects of the following drugs:

Antipyretics - Paracetamol (with synthesis and mode of action); Analgesics- Ibuprofen (with synthesis and overview of the mode of action); Antimalarials - Chloroquine (synthesis and mode of action).

An elementary treatment of Antibiotics and detailed study of chloramphenicol including mode of action. Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

## UNIT-3: UV-Vis and IR Spectroscopy

(Hours: 12)

UV-Vis and IR Spectroscopy and their application to simple organic molecules. Electromagnetic radiations and their properties; double bond equivalence and hydrogen deficiency. UV-Vis spectroscopy (electronic spectroscopy): General electronic transitions,  $\lambda_{\max}$  &  $\epsilon_{\max}$ , chromophores & auxochromes, bathochromic & hypsochromic shifts. Application of Woodward rules for the calculation of  $\lambda_{\max}$  for the following systems: conjugated dienes - alicyclic, homoannular and heteroannular;  $\alpha, \beta$ -unsaturated aldehydes and ketones, charge transfer complex.

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

## Practical component

Credit:02

(Laboratory periods: 15 classes of 4 hours each)

1. Isolation and estimation of the amount of aspirin in a commercial tablet.
2. Synthesis of ibuprofen.
3. Systematic qualitative identification and derivative preparation of organic compounds (Aromatic hydrocarbons, Aryl halides)
4. Detection of simple functional groups through examination of IR spectra (spectra to be provided). IR spectra of simple compounds like phenols, aldehydes, ketones, carboxylic acids may be given.
5. Differentiation between o-/p-hydroxybenzaldehyde by IR spectroscopy (Spectra to be provided).
6. Differentiation between benzoic acid and cinnamic acid by UV spectroscopy.
7. Laboratory preparation of paracetamol.
8. Diel's Alder reaction using Anthracene and Maleic anhydride.

## References:

### Theory:

1. Finar, I. L. **Organic Chemistry** (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Bahl, A; Bahl, B. S. (2012), **Advanced Organic Chemistry**, S. Chand.
4. Pavia, D.L. **Introduction to Spectroscopy**, Cengage learning (India) Pvt. Ltd.
5. Kemp, W. (1991), **Organic Spectroscopy**, Palgrave Macmillan.

### Practicals

1. Ahluwalia, V.K.; Dhingra, S.; Gulati, A. (2005), **College Practical Chemistry**, University Press (India) Ltd.
2. Ahluwalia, V.K.; Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
3. Vogel, A.I. (1972), **Textbook of Practical Organic Chemistry**, Prentice-Hall.
4. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.
5. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.

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## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE 9: Computer Applications in Chemistry

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE 9: Computer Applications in Chemistry</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

The Learning Objectives of this course are as follows:

- To introduce the students to basic computer skills that will help them in solving chemistry problems using spreadsheets and BASIC language.
- To acquaint the students with different software for data tabulation, calculation, graph plotting, data analysis and document preparation.
- To expose the students to the concept of molecular modelling, its applications to various molecular systems, energy minimization techniques, analysis of Mulliken Charge and ESP Plots.

### Learning outcomes

By studying this course, students will be able to:

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

### Syllabus

#### Unit 1: Programming using BASIC

(Hours: 20)

Programming Language – Elements of BASIC language, Numeric and string Constants and Variables, arithmetic expressions, hierarchy of operations, inbuilt functions. Syntax and use of the various QBASIC commands: REM, CLS, INPUT, PRINT, GOTO, IF, IF...THEN, IF...THEN..ELSE, IF and END IF, FOR

and NEXT etc., DIM, READ, DATA, GOSUB, RETURN, RESTORE, DEF FNR and Library Functions, Simple programs based on usage of the commands mentioned above.

Statistical analysis using BASIC: Mean, Least square fit - Linear regression, variance, standard deviation.

## **Unit 2 : Handling of Numerical Data**

**(Hours: 4)**

Spreadsheet software: MS Excel. Creating a spreadsheet, entering and formatting information, applying basic functions and formulae to the data, drawing charts, tables and graphs, displaying the equation of graph along with the  $R^2$  value, incorporating tables and graphs in Word files, graphical solution of equations, plotting pressure-volume curves of van der Waals gases, Maxwell-Boltzmann distribution, concentration versus time graphs, spectral data, titration curves, etc.

## **Unit 3: Molecular Modelling**

**(Hours: 6)**

Introduction to molecular modelling, overview of classical and quantum mechanical methods (molecular mechanics, semi empirical, ab initio and DFT), general considerations and comparison of these methods.

### **Practical component**

**Credit:02**

**(Laboratory periods: 15 classes of 4 hours each)**

### **Exercises of Programing**

1. Calculate pressure of a real gas using Van der Waal's Equation.
2. Calculate the most probable speed, average speed and root mean square velocity of an ideal gas.
3. Roots of quadratic equations
4. Binomial coefficient using GOSUB statement.
5. Mean, standard deviation
6. Least square curve fitting method for linear equation.

### **Plotting graphs using a spreadsheet**

1. Van der Waals isotherms
2. Maxwell-Boltzmann distribution curves as function of temperature and molecular weight
3. Plot the conductometric titration curve for
  - a) strong acid vs strong base and b) weak acid vs strong base
4. Plot the pH metric titration curve for
  - a) strong acid vs strong base and b) weak acid vs strong base and determine the  $pK_a$  of the weak acid
5. Plot the graphs for the kinetics of first order reaction and determine the rate constant
6. Plot the UV-vis absorbance spectra and determine the molar absorption coefficient.

### **Molecular Modelling**

1. Optimize and compare the geometry parameters of  $H_2O$  and  $H_2S$  using ArgusLab.
2. Compare the basicities of N atom in ammonia, methylamine, dimethylamine and trimethylamine using ArgusLab by comparing Mulliken charges and ESP map in ArgusLab.



3. Compare C-C bond lengths and bond order in ethane, ethene and ethyne using ArgusLab.
4. Determine enthalpy of isomerization of cis and trans-2-butene using ArgusLab.
5. Compare the HAH bond angles for the second row hydrides ( $\text{BeH}_2$ ,  $\text{CH}_4$ ,  $\text{NH}_3$ ,  $\text{H}_2\text{O}$ ) and compare with the results from qualitative MO theory.

## References:

### Theory:

1. Levie, R. de. (2001), **How to use Excel in analytical chemistry and in general scientific data analysis**, Cambridge Univ. Press.
2. Venit, S.M. (1996), **Programming in BASIC: Problem solving with structure and style**. Jaico Publishing House.
3. Lewars, E. (2003), **Computational Chemistry**, Kluwer academic Publisher.
4. Cramer, C.J.(2004), **Essentials of Computational Chemistry**, John Wiley & Sons.
5. Hinchcliffe, A. (1996), **Modelling Molecular Structures**, John Wiley & Sons.
6. Leach, A.R.(2001), **Molecular Modelling**, Prentice-Hall.

### Practicals

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

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## SEMESTER VI

### DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -10: Analytical Methods in Chemistry

#### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE-10: Analytical Methods in Chemistry</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

#### Learning Objectives

The Learning Objectives of this course are as follows:

- To familiarize students with the concepts of sampling, errors in analysis, accuracy, precision and introduce basics of statistical analysis.
- To introduces students to important instrumentation and separation techniques routinely used in the laboratory analysis of samples. The experiments expose students to instrumentation and they learn to detect and separate analytes in a mixture.

#### Learning outcomes

By studying this course, students will be able to:

- Understand various sources of errors in chemical analysis.
- Learn about methods to minimize error.
- Understand basic principle of instrumentation (Flame Photometer, UV-vis spectrophotometer, Atomic Absorption spectrophotometer).
- Apply the principles of analysis and instrumentation to analyse soil samples, soft drinks and synthetic mixtures provided in the laboratory.
- Learn basic principles of separation techniques (chromatography and solvent extraction) and apply them to separate mixtures.
- Understand principles of Gravimetric analysis and apply them in determination of  $\text{Ni}^{2+}$  and  $\text{Al}^{3+}$
- Analyse samples independently in the laboratory.

#### Syllabus

Unit 1: Errors in Chemical Analysis

(Hours: 8)

Types of errors, Accuracy and Precision, Absolute and relative uncertainty, propagation of uncertainty. The Gaussian distribution, mean and standard deviation, confidence intervals.

## **Unit 2: Optical Methods of Analysis**

**(Hours: 10)**

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

### ***UV-Vis Spectrophotometry***

Basic principles of instrumentation for single and double beam instruments. Determination of concentration of unknown compounds, composition of metal complexes using Job's method of continuous variation and mole ratio method.

### ***Flame Atomic Absorption and Emission Spectroscopy***

Basic principles of instrumentation. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal.

Application of these techniques in analysis of samples.

## **Unit 3: Separation Techniques**

**(Hours: 12)**

### ***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.

### ***Chromatography***

Principles of Chromatographic separations, Classification of Chromatographic techniques, Thin Layer Chromatography, Column Chromatography, efficiency of separation (Resolution, Efficiency of Resolution, Plate Height) Application of these techniques in analysis of samples.

## **Practical Component**

**Credits:02**

### **(Laboratory periods:60)**

1. Analysis of soil.
  - a. Determination of pH of soil, Total soluble salts, carbonate and bicarbonate, calcium and magnesium by titration.
  - b. Estimation of Potassium, calcium and magnesium by flame photometry.
2. Separation of constituents of leaf pigments by thin layer chromatography.
3. Determination of the ion exchange capacity of an anion exchange resin.
4. Determination of the ion exchange capacity of a cation exchange resin.
5. Separation of amino acids by ion exchange chromatography.

6. Spectrophotometric analysis of  $\text{Co}^{2+}$  and  $\text{Ni}^{2+}$  ions in a mixture.
7. Spectrophotometric analysis of Caffeine and Benzoic acid in a soft drink.
8. Gravimetric estimation of  $\text{Ni}^{2+}$  using Dimethylglyoxime or  $\text{Al}^{3+}$  using oxine.

#### References:

#### Theory:

1. Willard, H.H. (1988), **Instrumental Methods of Analysis**, 7th Edition, Wardsworth Publishing Company.
2. Christian, G.D. (2004), **Analytical Chemistry**, 6th Edition, John Wiley & Sons, New York.
3. Harris, D. C. (2007), **Quantitative Chemical Analysis**, 6th Edition, Freeman.
4. Skoog, D.A.; Holler F.J.; Nieman, T.A. (2005), **Principles of Instrumental Analysis**, Thomson Asia Pvt. Ltd.
5. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989), **Vogel's Textbook of Quantitative Chemical Analysis**, John Wiley and Sons.

#### Practicals:

1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989), **Vogel's Textbook of Quantitative Chemical Analysis**, John Wiley and Sons.
2. Christian, G.D. (2004), **Analytical Chemistry**, 6th Edition, John Wiley & Sons, New York.
3. Harris, D. C. (2007), **Quantitative Chemical Analysis**, 6th Edition, Freeman.
4. Skoog, D.A.; Holler F.J.; Nieman, T.A. (2005), **Principles of Instrumental Analysis**, Thomson Asia Pvt. Ltd.

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## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE 11: Chemistry of Polymers, Dyes and Natural Products

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE 11: Chemistry of Polymers, Dyes and Natural Products</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

The Learning Objectives of this course are as follows:

- To understand the process of converting knowledge of chemistry into marketable products for commercial gain.
- To familiarize the basic nomenclature of polymers, dyes and natural products, classification and important terms.

### Learning outcomes

By studying this course, students will be able to:

- Learn about the chemistry of natural and synthetic polymers including fabrics and rubbers.
- Understand the chemistry of biodegradable and conducting polymers and appreciate the need of biodegradable polymers with emphasis on basic principles.
- Comprehend the theory of colour and constitution as well as the chemistry of dyeing.
- Know applications of various types of dyes including those in foods and textiles.
- Understand the chemistry and applications of natural products like terpenoids and alkaloids.

### Syllabus

#### Unit 1: Polymers

**(Hours: 12)**

Introduction and classification based on origin, monomer units, thermal response, mode of formation, structure, application and tacticity; di-block, tri-block and amphiphilic polymers;

Weight average molecular weight, number average molecular weight, glass transition temperature ( $T_g$ ) of polymers; Polymerisation Reactions-Addition and condensation. Mechanism of cationic, anionic and free radical addition polymerization; Ziegler-Natta polymerisation of alkenes.

Preparation and applications of: Plastics -thermosetting (phenol-formaldehyde, polyurethanes) and thermosoftening(PVC, polythene); Fabrics -natural (cellulose and synthetic derivatives of cellulose like rayon and viscose); synthetic (acrylic, polyamide, polyester); Rubbers-natural

and synthetic: Buna-N, Buna-S, Neoprene, silicon rubber; Vulcanization; Polymer additives; Introduction to Specialty Polymers: electroluminescent (Organic light emitting diodes), conducting, biodegradable polymers and liquid crystals.

## **Unit 2: Dyes**

**(Hours: 8)**

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing. Synthesis and applications of Azo dyes – Methyl orange, Congo red; Triphenyl methane dyes- Crystal violet; Phthalein Dyes – Phenolphthalein; Natural dyes –Structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

## **Unit 3: Natural Product Chemistry- An Introduction to Terpenoids and Alkaloids**

**(Hours: 10)**

Terpenes: Introduction, occurrence, classification, uses, isoprene and special isoprene rule; structure elucidation, synthesis and industrial application of citral.

Alkaloids: Introduction, occurrence, classification, uses, general structural features, general methods for structure elucidation including Hoffmann's exhaustive methylation and Emde's method. Structure elucidation, synthesis and physiological action of Nicotine.

## **Practical component**

**Credits: 02**

### **(Laboratory periods: 60)**

1. Preparation of Methyl Orange.
2. Preparation of Malachite Green.
3. Recycling of Plastic: Moulding of plastic or Cracking of plastic.
4. Preparation of Urea-formaldehyde resin.
5. Preparation of Methyl Orange.
6. (a) Dyeing of different fabrics (cotton, wool, silk) using Alizarin or any other dye.
7. (b) Preparation of azo dye on the surface of the fabric.
8. Qualitative test for identification of alkaloids (Dragendorff's reagent and Mayer's reagent test) and terpenoids (Salkowski test).
9. Preparation of perchromic dye using p-amino phenol and p-nitro benzaldehyde.

## **References:**

### **Theory:**

1. Finar, I.L. (2008), **Organic Chemistry**, Vol 2, 5th Edition, Pearson Education

2. Saunders, K. J. (1988), **Organic Polymer Chemistry**, 2nd Edition Chapman & Hall, London
3. Campbell, Ian M., (2000), **Introduction to Synthetic Polymers**, 2nd Edition Oxford University Press, USA.
4. Bahadur, P. and Sastry, N.V. (2002) **Principles of Polymer Science**, Narosa, New Delhi
5. Patrick, G. **An Introduction to Medicinal Chemistry** (2013), 4th Edition, Oxford University Press.
6. Priscilla Abarca, Patricia Silva, Iriux Almodovar and Marcos Caroli  
ezende\*Quim. Nova, Vol. 37, No. 4, 745-747, 2014.  
<http://dx.doi.org/10.5935/0100-4042.20140120>

**Practical:**

1. Furniss B S., Hannaford A. J., Smith Peter W. G. & Tatchell Austin R., **Vogel's Textbook of Practical Organic Chemistry** Fifth Edition, Longman Scientific & Technical.
2. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.

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## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -12: Phase Equilibria and Photochemistry

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Chem-DSE 12: Phase Equilibria and Photochemistry</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

The Learning Objectives of this course are as follows:

- To develop basic understanding of Phase, Component, Degree of freedom, basic principles of phase equilibria,
- To understand phase diagram of one and two component systems.
- The students will also gain an understanding of Binary solution, distillation of binary solution, CST and distribution law & its applications.

### Learning outcomes

By studying this course, students will be able to:

- Understand phase equilibrium, criteria, CST, Gibbs-Duhem-Margules equation.
- Apply the concepts of phase, conductance and distribution law while studying other chemistry courses and every-day life.
- Explain low and high quantum yield, photosensitized reactions

### Syllabus

#### Unit 1: Phase Equilibria

**(Hours: 22)**

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, Phase diagram for one component systems ( $H_2O$  and S). Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points.



Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non-ideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications.

## Unit 2: Photochemistry

(Hours: 8)

Characteristics of electromagnetic radiation. Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws of photochemistry, quantum yield, examples of low and high quantum yields

Photosensitized reactions, Jablonski's diagram. Role of photochemical reactions in biochemical processes, chemiluminescence.

## Practical component

Credits: 02

### (Laboratory periods: 60)

#### *Phase Equilibrium*

1. Determination of critical solution temperature and composition at CST of the phenol water system.
2. Effect of impurity on CST of phenol-water system (NaCl and succinic acid).
3. Construction of the phase diagram using cooling curves :
  - a. Simple eutectic.
  - b. Congruent melting system(s).
4. Distribution of acetic/ benzoic acid between water and chloroform or cyclohexane.
5. Study of equilibrium of any one of the following reactions by distribution method:
  - (i)  $I_2(aq) + I^-(aq) \rightleftharpoons I_3^-(aq)$
  - (ii)  $Cu^{2+}(aq) + nNH_3 \rightleftharpoons [Cu(NH_3)_n]^{2+}$

## References:

### Theory:

1. Atkins, P.W.; Paula, J.de. (2014), **Atkin's Physical Chemistry Ed.**, 10th Edition, Oxford University Press.
2. Ball, D. W. (2017), **Physical Chemistry**, 2nd Edition, Cengage Learning, India.
3. Castellan, G. W. (2004), **Physical Chemistry**, 4th Edition, Narosa.
4. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 1, 6th Edition, McGrawHill Education.
5. Kapoor, K.L., **A Textbook of Physical Chemistry**, Vol 3, 5th Edition, McGraw Hill Education.

### Practical:

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), **Senior Practical Physical Chemistry**, R.Chand & Co, New Delhi.
2. Kapoor, K.L. (2019), **A Textbook of Physical Chemistry**, Vol.7, 1st Edition, McGrawHill Education.
3. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P. (2003), **Experiments in Physical Chemistry**, 8th Edition, McGraw-Hill, New York

**Additional Resources:**

1. Moore, W.J. (1972), **Physical Chemistry**, 5th Edition, Longmans Green & Co. Ltd.
2. Glasstone, S. (1948), **Textbook of Physical Chemistry**, D. Van Nostrand company, New York.

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## DISCIPLINE SPECIFIC ELECTIVE COURSE – 13 (DSE-13): Research Methodology for Chemists

### CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>Research Methodology for Chemists (DSE-13)</b>	04	03	--	01	Class 12 <sup>th</sup> with Physics, Chemistry	

### Learning objectives

The objectives of this course are as follows:

- To make the students aware of fundamental but mandatory ethical practices in chemistry.
- To introduce the concept of data analysis.
- To learn to perform literature survey in different modes.
- To make the students aware of safety handling and safe storage of chemicals.
- To make students aware about plagiarism and how to avoid it.
- To teach the use of different e-resources.

### Learning outcomes

By studying this course, students will be able to:

- Follow ethical practices in chemistry
- Do Data analysis
- Literature survey in different modes
- Use e-resources.
- Avoid plagiarism, understand the consequences and how to avoid

## SYLLABUS OF DSE-13

### UNIT – 1: Scope of Research

(Hours: 3)

Introduction, overview of research process: define research problem, review literature, formulate hypothesis, design research/experiment, collect and analyse data, interpret and report, scope and importance.

### UNIT – 2: Literature Survey, Databases and Research metrics

(Hours: 15)

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, Digital: Databases and their responsible use: Google Scholar, Web of science, Scopus, UGC INFONET, SciFinder, PubMed, ResearchGate, E-consortium, e-books; Search techniques: Phrase, Field, Boolean, Proximity, Concept, Limiting/Refining Search Results. Research metrics: Impact factor of Journal, h-index, i10 index, Altmetrics, Citation index. Author identifiers/or profiles: ORCID, Publons, Google Scholar, ResearchGate, VIDWAN

### **UNIT – 3: Communication in Science**

**(Hours: 12)**

Types of technical documents: Full length research paper, book chapters, reviews, short communication, project proposal, Letters to editor, and thesis.

Thesis writing – different steps and software tools (Word processing, LaTeX, Chemdraw, Chems sketch etc) in the design and preparation of thesis, layout, structure (chapter plan) and language of typical reports, Illustrations and tables, bibliography, referencing: Styles (APA, Oxford etc), annotated bibliography, Citation management tools: Mendeley, Zotero and Endnote; footnotes. Oral presentation/posters – planning, software tools, creating and making effective presentation, use of visual aids, importance of effective communication, electronic manuscript submission, effective oral scientific communication and presentation skills.

### **UNIT – 4: Research and Publication ethics**

**(Hours: 9)**

Scientific Conduct: Ethics with respect to science and research, Scientific Misconducts: falsification, fabrication and plagiarism, similarity index, software tools for finding plagiarism (Turnitin, Urkund etc), redundant publications

Publication Ethics: Introduction, COPE (Committee on Publication Ethics) guidelines; conflicts of interest, publication misconduct: problems that lead to unethical behaviour and vice versa, types, violation of publication ethics, authorship and contributorship, predatory publishers and journals

IPR - Intellectual property rights and patent law, commercialization, copy right, royalty, trade related aspects of intellectual property rights (TRIPS)

### **UNIT – 5: Statistical analysis for chemists** **6)**

**(Hours:**

Types of data, data collection-Methods and tools, data processing, hypothesis testing, Normal and Binomial distribution, tests of significance: t-test, F-test, chi- square test, ANOVA, multiple range test, regression and correlation.

Features of data analysis with computers and softwares -Microsoft Excel, Origin, SPSS

### **Practical component**

**Credits: 01**

**(Laboratory periods:15 classes of 2 hours each)**

1. Collection of journal articles on a particular topic using Google Scholar and creating a database.
2. Collection of journal articles on a particular topic using Science Direct and creating a database.
3. Collection of journal articles on a particular topic using Scopus and creating a database.
4. Drawing chemical structure, reactions and mechanisms using Chems sketch or ISIS draw or any other software.

5. Collection of chemical structure using ChemSpider and creating a database.
6. Curve fitting using freely available softwares/apps (any one)
7. Making of power point presentation
8. Experimental learning of safe storage hazardous chemicals
9. Experimental learning of handling of hazardous chemicals
10. Technical writing on topics assigned.
11. Demonstration for checking of plagiarism using recommended software

**Essential/recommended readings:**

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