## DEPARTMENT OF CHEMISTRY

BSc. (Hons.) Chemistry

*Category-I*

**DISCIPLINE SPECIFIC CORE COURSE -1 (DSC-1): Atomic Structure & Chemical Bonding**

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

| Course t itle & Code | Credits | Credit distribution of the course | | | Eligibility criteria | Pre-requisite o f the course (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Atomic Structure & Chemical Bonding (DSC-1: Inorganic Chemistry -I) | 04 | 03 | — | 01 | Physics, Chemistry, Mathematics | -- |

### Learning Objectives

The course reviews the structure of the atom, which is a necessary pre-requisite in understanding the nature of chemical bonding in compounds. It provides basic knowledge about ionic and covalent bonding, and explains that chemical bonding is best regarded as a continuum between the two cases. It discusses the periodicity in properties with reference to the s and p block, which is necessary in understanding their group chemistry. The student will also learn about the fundamentals of acid-base and redox titrimetric analysis.

### Learning outcomes

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

- Solve the conceptual questions using the knowledge gained by studying the quantum mechanical model of the atom, quantum numbers, electronic configuration, radial and angular distribution curves, shapes of s, p, and d orbitals, and periodicity in atomic radii, ionic radii, ionization enthalpy and electron affinity of elements.
- Draw the plausible structures and geometries of molecules using radius ratio rules, VSEPR theory and MO diagrams (homo- & hetero-nuclear diatomic molecules).
- Understand the concept of lattice energy using Born-Landé and Kapustinskii equation.
- Calibrate the apparatus used in titrimetric analysis and prepare standard solutions for titration
- Understand the theory and application of various acid-base and redox titrations.
- Comprehend the theory of acid-base indicators

## SYLLABUS OF DSC-1

**UNIT – I (15 Hours)**
Unit 1: Atomic Structure

Recapitulation of concept of atom in ancient India, Bohr's theory & its limitations, atomic spectrum of hydrogen atom.

de Broglie equation, Heisenberg's Uncertainty Principle and its significance. Postulates of wave mechanics, Time independent Schrödinger's wave equation, well behaved wave function, significance of $\psi$ and $\psi^2$. Quantum mechanical treatment of H- atom, Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial function plots, radial probability distribution plots, angular distribution curves. Shapes of *s*, *p*, and *d o*rbitals, Relative energies of orbitals.

Pauli's Exclusion Principle, Hund's rule of maximum spin multiplicity, Aufbau principle and its limitations.

**UNIT – II (6 Hours)**

**Unit 2: Periodic properties of Elements & Periodic Trends**

Brief discussion of the following properties of the elements, with reference to *s*- & *p*-block andtheir trends:

(a) Effective nuclear charge, shielding or screening effect and Slater's rules

(b) Atomic and ionic radii

(c) Ionization enthalpy (Successive ionization enthalpies)

(d) Electron gain enthalpy

(e) Electronegativity, Pauling's scale of electronegativity. Variation of electronegativity with bond order and hybridization.

**UNIT – III (12 Hours)**

**Unit 3: Ionic bond**

General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Lattice energy, Born-Landé equation with derivation, Madelung constant, importance of Kapustinskii equation for lattice energy. Born-Haber cycle and its applications.

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

**UNIT – IV (12 Hours)**
**Unit 4: Covalent bond**
Valence shell electron pair repulsion (VSEPR) theory, shapes of the following simple molecules and ions containing lone pairs and bond pairs of electrons: $H_2O$, $NH_3$, $PCl_3$, $PCl_5$,

$SF_6$, $ClF_3$, $I_3$, $BrF_2^+$, $PCl_6^-$, $ICl_2^-$ $ICl_4^-$, and $SO_4^{2-}$. Application of VSEPR theory in predicting trends in bond lengths and bond angles.

Valence Bond theory (*Heitler-London* approach). Hybridization, equivalent and non-equivalent hybrid orbitals, Bent's rule.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

Molecular orbital diagrams of homo & hetero diatomic molecules [$N_2$,$O_2$, $C_2$, $B_2$, $F_2$, CO, NO] and their ions; HCl (idea of s-p mixing and orbital interaction to be given).

**Practical component**
**Practicals: Inorganic Chemistry-I** **(30 Hours)**

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

1. **Titrimetric Analysis:**
   (i) Calibration and use of apparatus
   (ii) Preparation of solutions ofdifferent Molarity/Normality.

2. **Acid-Base Titrations:** Principles of acid-base titrations to be discussed.
(i) Estimation of oxalic acid using standardized NaOH solution
(ii) Estimation of sodium carbonate using standardized HCl.
(iii) Estimation of carbonate and hydroxide present together in a mixture.
(iv) Estimation of carbonate and bicarbonate present together in a mixture.

3. **Redox Titration:** Principles of oxidation-reduction titrations to be discussed.
(i) Estimation of oxalic acid using standardized $KMnO_4$ solution
(ii) Estimation of water of crystallization in Mohr's salt by titrating with $KMnO_4$.
(iii) Estimation of oxalic acid and sodium oxalate in a given mixture.

**Essential/recommended readings**
**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. Pfennig, B. W. (2015), **Principles of Inorganic Chemistry.** John Wiley & Sons.
6. Housecraft, C. E.; Sharpe, A. G., (2018), Inorganic Chemistry, 5th Edition, Pearson.
7. Wulfsberg, G (2002), **Inorganic Chemistry,** Viva Books Private Limited.
8. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), **Inorganic Chemistry**, 5th Edition, Pearson.

9. Shiver, D.; Weller, M.; Overton, T.; Rourke, J.; Armstrong, F. (2014), **Inorganic Chemistry**, 6th Edition, Freeman & Company
10. Das, A. K.; Das, M. (2014), **Fundamental Concepts of Inorganic Chemistry**, 1st Edition, Volume CBS Publishers & Distributors Pvt. Ltd.

**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. Harris, D. C.; Lucy,C. A.(2016), **Quantitative Chemical Analysis,** 9th Edition, Freeman andCompany

**Note: E xamination s cheme a nd m ode s hall be a s pr escribed by t he E xamination Branch, University of Delhi, from time to time.**

## DISCIPLINE SPECIFIC CORE COURSE – 2 (DSC-2): Basic Concepts and Aliphatic Hydrocarbons

**Credit distribution, Eligibility and Prerequisites of the Course**

| Course t itle & Code | Credits | Credit distribution of the course | | | Eligibility criteria | Pre-requisite of the course (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Basic Concepts and Aliphatic Hydrocarbons (DSC-2: Organic Chemistry-I) | **04** | **03** | **--** | **01** | Physics, Chemistry, Mathematics | **--** |

**Learning Objectives**

The core course Organic Chemistry I is designed in a manner that it forms a cardinal part of the learning of organic chemistry for the subsequent semesters. The course is infused with the recapitulation of fundamental concepts 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, the functional groups-alkanes, alkenes, alkynes are introduced. The constitution of the course strongly aids in the paramount learning of the concepts and their applications.

**Learning outcomes**

**On completion of the course, the student will be able to:**

- Understand and explain the electronic displacements and reactive intermediates and their applications in basic concepts.
- Formulate the mechanistic route of organic reactions by recalling and correlating the fundamental concepts.

- Identify and comprehend mechanism for free radical substitution, electrophilic addition, nucleophilic substitution and elimination reactions.
- Understand the fundamental concepts of stereochemistry.
- Understand and suitably use the chemistry of hydrocarbons

**SYLLABUS OF DSC- 2**

**UNIT – I ( 9 Hours)**
**Unit I: Basic Concepts of Organic Chemistry**

Electronic displacements and their applications: inductive, electromeric, resonance and mesomeric effects and hyperconjugation. Dipole moment, acidity and basicity.

Homolytic and heterolytic fissions with suitable examples. Types, shape and relative stability of carbocations, carbanions, carbenes and free radicals.

Electrophiles & nucleophiles, and introduction to types of organic reactions: addition, elimination and substitution reactions.

**UNIT – II (18 Hours)**
**Unit II: Stereochemistry**

Stereoisomerism: Optical activity and optical isomerism, asymmetry, chirality, enantiomers, diastereomers. specific rotation; Configuration and projection formulae: Newman, Sawhorse, Fischer and their interconversion. Chirality in molecules with one and two stereocentres; meso configuration.

Racemic mixture and their resolution. Relative and absolute configuration: D/L and R/S designations (CIP rules).

Geometrical isomerism: *cis-trans, syn-anti* and *E/Z* notations.

Conformational Isomerism: Alkanes (Conformations, relative stability and energy diagrams of Ethane, Propane and butane). Relative stability of cycloalkanes (Baeyer strain theory), Cyclohexane conformations with energy diagram. Conformations of monosubstituted cyclohexanes.

**UNIT – III (18)**
**Unit III: Aliphatic Hydrocarbons**

Alkanes: Preparation, Halogenation of alkanes, Concept of relative reactivity v/s selectivity.

Alkenes and Alkynes: Methods of preparation of alkenes using Mechanisms of E1, E2, E1cb reactions, Saytzeff and Hoffmann eliminations. Electrophilic additions, mechanism with suitable examples, (Markownikoff/Anti-markownikoff addition), *syn* and *anti*-addition; addition of $H_2$, $X_2$, oxymercuration-demercuration, hydroboration-oxidation, ozonolysis, hydroxylation, reaction with NBS, Reactions of alkynes; acidity, Alkylation of terminal alkynes, electrophilic addition: hydration to form carbonyl compounds, Relative reactivity of alkenes and alkynes, 1,2-and 1,4-addition reactions in conjugated dienes, Diels Alder reaction (excluding stereochemistry)

**Practical component**

**Practical (30 Hours)**
**Credits: 01**

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

**Note:** *Students should be provided with handouts prior to the practical class*

1. Calibration of a thermometer and determination of the melting points of the organic compounds using any one of the following methods-Kjeldahl method, electrically heated melting point apparatus and BODMEL).

2. Concept of melting point and mixed melting point.

3. Concept of recrystallisation using alcohol/water/alcohol-water systems (Any two).
4. Determination of boiling point of liquid compounds (boiling point lower than and more than 100 °C by distillation, capillary method and BODMEL method)

5. Separation of a mixture of two amino acids/sugars by radial/ascending paper chromatography.

6. Separation of a mixture of *o*-and *p*-nitrophenol or *o*-and *p*-aminophenol by thin layer chromatography (TLC).

7. Detection of extra elements

**Essential/recommended readings**

**References:**

**Theory**


1. Morrison, R.N., Boyd, R.N., Bhattacharjee, S.K. (2010), **Organic Chemistry**, 7th Edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
2. Finar, I.L. (2002), **Organic Chemistry**, Volume 1, 6th Edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
3. Eliel, E.L., Wilen, S.H. (1994), **Stereochemistry of Organic Compounds**; Wiley: London.


**Practicals**


1. Mann, F.G., Saunders, B.C. (2009), **Practical Organic Chemistry**, 4th Edition, Pearson Education.
2. Ahluwalia, V.K., Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
3. Furniss, B.S., Hannaford, A.J., Smith, P.W.G.; Tatchell, A.R (2004), **Vogel's Textbook of Practical Organic Chemistry**, Pearson.
4. Leonard, J., Lygo, B., Procter, G. (2013) **Advanced Practical Organic Chemistry**, 3rd Edition, CRC Press.
5. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi

**Suggestive readings**

**Additional Resources:**


1. Solomons, T.W.G., Fryhle, C.B., Snyder, S.A. (2017), **Organic C hemistry**, 12th Edition, Wiley.
2. Bruice, P.Y. (2020), **Organic Chemistry**, 8th Edition, Pearson.
3. Clayden, J., Greeves, N., Warren, S. (2014), **Organic Chemistry**, Oxford.
4. Nasipuri, D. (2018), **Stereochemistry o f O rganic C ompounds: P rinciples a nd Applications**, 4th Edition, New Age International.
5. Gunstone, F.D. (1975), **Guidebook to Stereochemistry**, Prentice Hall Press.
6. Gupta, S.S. (2018), **Basic S tereochemistry o f O rganic Mo lecules,** 2nd Edition, Oxford University Press.


## DISCIPLINE SPECIFIC CORE COURSE– 3 (DSC-3): Gaseous and Liquid

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

| Course t itle & Code | Credits | Credit distribution of the course | | | Eligibility criteria | Pre-requisite of t he co urse (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Gaseous and Liquid State (DSC-3: Physical Chemistry-I) | **04** | **02** | **--** | **02** | Physics, Chemistry, Mathematics | **--** |

**Learning Objectives**

The objective of this course is to develop basic and advance concepts regarding gases and liquids. It aims to study the similarity and differences between the two states of matter and reasons responsible for these. The objective of the practicals is to develop skills for working in physical chemistry laboratory. The student will perform experiments based on the concepts learnt in Physical chemistry-I course.

**Learning outcomes**

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

- Derive mathematical expressions for different properties of gas and liquid and understand their physical significance.
- Apply the concepts of gas equations and liquids while studying other chemistry courses and every-day life.
- Handle stalagmometer and Ostwald viscometer properly.
- Determine the density of aqueous solutions.
- Dilute the given solutions as per required concentrations.
- Data reduction using numerical and graphical methods.

**SYLLABUS OF DSC-3**

**UNIT – I (24 Hours)**
**Gaseous state**

**Kinetic theory of gases-** postulates and derivation of kinetic gas equation, Maxwell distribution of molecular velocities and its use in evaluating average, root mean square and most probable velocities and average kinetic energy. Definition, expression, applications and temperature and pressure dependence of each one of the following properties of ideal gases: Collision frequency, Collision diameter, Mean free path. Coefficient of viscosity, definition, units and origin of viscosity of gases, relation between mean free path and coefficient of viscosity, temperature and pressure dependence of viscosity of a gas, calculation of molecular diameter from viscosity
Barometric distribution law, its derivation and applications, alternative forms of barometric distribution law in terms of density and number of molecules per unit volume, effect of height, temperature and molecular mass of the gas on barometric distribution

**Behaviour of real gases-** Compressibility factor, Z , Variation of compressibility factor with pressure at constant temperature *(plot of Z vs P)* for different gases ( $H_2$, $CO_2$, $CH_4$ and $NH_3$), Cause of deviations from ideal gas behaviour and explanation of the observed behaviour of real gases in the light of molecular interactions

**van der Waals (vdW) equation of state,** Limitations of ideal gas equation of state and its modifications in the form of derivation of van der Waal equation, Physical significance of van der Waals constants, application of van der Waal equation to explain the observed behaviour of real gases.

**Isotherms of real gases-** Critical state, relation between critical constants and van der Waals constants, correlation of critical temperature of gases with intermolecular forces of attraction, Continuity of states, Limitations of van der Waals equation, Reduced equation of state and law of corresponding states (statement only).

**Virial equation of state-**Physical significance of second and third virial coefficients, van der Waals equation expressed in virial form, Relations between virial coefficients and van der Waals constants

**UNIT – II (6 Hours)**
**Liquid state**

Nature of liquid state, qualitative treatment of the structure of the liquid state

Physical properties of liquids-vapour pressure, its origin and definition, Vapour pressure of liquids and intermolecular forces, and boiling point

Surface tension, its origin and definition, Capillary action in relation to cohesive and adhesive forces, determination of surface tension by (i) using stalagmometer (drop number and drop mass method both) and (ii) capillary rise method, Effects of addition of sodium chloride, ethanol and detergent on the surface tension of water and its interpretation in terms of molecular interactions, Role of surface tension in the cleansing action of detergents

Coefficient of viscosity and its origin in liquids, Interpretation of viscosity data of pure liquids (water, ethanol, ether and glycerol) in the light of molecular interactions, Effects of addition of sodium chloride, ethanol and polymer on the viscosity of water, relative viscosity, specific viscosity and reduced viscosity of a solution, comparison of the origin of viscosity of liquids and gases, effect of temperature on the viscosity of a liquid and its comparison with that of a gas.

**Practical component**
**Practicals** **60 Hours**

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

**1. Gases**

a. To verify the Charles law using Charles law apparatus
b. To determine the value of universal gas constant R using the reaction
$Mg(s) + 2HCl\ (aq) \rightarrow MgCl_2\ (aq) + H_2\ (g)$

**2. Surface tension measurements using stalagmometer**

a. Determine the surface tension of a liquid by drop number method.
b. Determine the surface tension of a liquid by drop weight method.
c. Study the variation of surface tension with different concentration of detergent solutions. Determine CMC.
d. Study the effect of the addition of solutes on the surface tension of water at room temperature and explain the observations in terms of molecular interactions:
(i) sugar
(ii) ethanol
(iii) sodium chloride
e. Study the variation of surface tension with different concentration of sodium chloride solutions.

**3. Viscosity measurement using Ostwald's viscometer**

a. Determination of co-efficient of viscosity of two unknown aqueous solution.
b. Study the variation of viscosity with different concentration of sugar solutions.
c. Study the effect of the addition of solutes such as (i) polymer (ii) ethanol (iii) sodium chloride on the viscosity of water at room temperature and explain the observations in terms of molecular interactions

d. Study the variation of viscosity of water with the amounts of a solute and calculate the intrinsic viscosity at room temperature.
e. Determine the viscosity average molecular mass of the polymer (PVA) using viscosity measurements.

**Essential/recommended readings**
**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, McGraw Hill Education.


**Practical:**


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


**Suggestive readings**

**Additional Resources:**


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

**DEPARTMENT OF CHEMISTRY**
**Category-I**

**B.Sc. (H) Chemistry**

## DISCIPLINE SPECIFIC CORE COURSE -4 (DSC-4): CHEMISTRY OF S- AND P-BLOCK ELEMENTS

### 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 | | |
| Chemistry of s- and p-Block Elements (DSC-4: Inorganic Chemistry -II) | 04 | 03 | 0 | 01 | Class 12$^{th}$ Pass | ---- |

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

- To develop the general principles of metallurgy and s-, p-block elements.
- To introduce the terms minerals, ores, concentration, benefaction, calcination, roasting, refining, etc. and explain the principles of oxidation and reduction as applied to the extraction procedures.
- To make students ware of different methods of purification of metals, such as electrolytic, oxidative refining, VanArkel-De Boer process and Mond's process are discussed and applications of thermodynamic concepts like that of Gibbs energy and entropy to the extraction of metals.
- To familiarize students with the patterns and trends exhibited by s- and p-block elements and their compounds with emphasis on synthesis, structure, bonding and uses.
- To impart information about the fundamentals of internal and external redox indicators, and iodometric/iodimetric titrations.

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

- Learn the fundamental principles of metallurgy and understand the importance of recovery of by-products during extraction.
- Applications of thermodynamic concepts like that of Gibbs energy and

entropy to the principles of extraction of metals.

- Learn about the characteristics of s- and p- block elements as well as the synthesis, structure, bonding and uses of their compounds
- Understand the concept and use of internal and external redox indicators
- Comprehend the theory and application of iodometric and iodimetric titrimetric analysis

**SYLLABUS OF DSC-4**

**UNIT – I: 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. Brief discussion of metals and alloys used in ancient and medieval India.

**UNIT – II**: **Chemistry of s- Block Elements** **(15 Hours)**

General characteristics: melting point, flame colouration, reducing nature, diagonal relationships and anomalous behavior of first member of each group. Reactions of alkali and alkaline earth metals with oxygen, hydrogen, nitrogen and water.

Common features such as ease of formation, thermal stability, energetics of dissolution, and solubility of the following alkali and alkaline earth metal compounds: hydrides, oxides, peroxides, superoxides, carbonates, nitrates, sulphates.

Complex formation tendency of s-block elements; structure of the following complexes: crown ethers and cryptates of Group I; basic beryllium acetate, beryllium nitrate, EDTA complexes of calcium and magnesium.

Solutions of alkali metals in liquid ammonia and their properties

**UNIT – III: Chemistry of *p*-Block Elements** **(9 Hours)**

Electronic configuration, atomic and ionic size, metallic/non-metallic character, melting point, ionization enthalpy, electron gain enthalpy, electronegativity, Catenation, Allotropy of C, P, S; inert pair effect, diagonal relationship between B and Si and anomalous behaviour of first member of each group.

**UNIT – IV: Compounds of *p*-Block Elements** **(15 Hours)**

Acidic/basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, action of heat on the following:

- Hydrides of Group 13 (only diborane), Group 14, Group 15 ($EH_3$ where E = N, P,As, Sb, Bi), Group 16 and Group 17.
- Oxoacids of phosphorus, sulphur and chlorine
- Interhalogen and pseudohalogen compound
- Clathrate compounds of noble gases, xenon fluorides (MO treatment of $XeF_2$).

**Practical component – 30 Hours**

1. **Redox Titrations**
   (i) Estimation of Fe(II) with $K_2Cr_2O_7$ using diphenylamine as internal indicator.
   (ii) Estimation of Fe(II) with $K_2Cr_2O_7$ using N-phenyl anthranilic acid as internal indicator.
   (iii) Estimation of Fe(II) with $K_2Cr_2O_7$ using external indicator.

2. **Iodo/Iodimetric Titrations**
   (i) Estimation of Cu(II) using sodium thiosulphate solution (Iodometrically).
   (ii) Estimation of $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodometrically).
   (iii) Estimation of antimony in tartaremetic iodimetrically.
   (iv) Estimation of Iodine content in iodized salt.

**Essential/recommended readings**

**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. 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.
4. Miessler, G. L.; Fischer P. J.; Tarr, D. A. (2014), **Inorganic Chemistry**, 5th Edition, Pearson.
5. Housecraft, C. E.; Sharpe, A. G., (2018), **Inorganic Chemistry**, 5thEdition, Pearson.
6. Canham, G. R., Overton, T. (2014), **Descriptive Inorganic Chemistry,** 6th Edition, Freeman and Company.
7. Greenwood, N. N.; Earnsaw, A., (1997), **Chemistry of Elements**, 2nd Edition, Elsevier.


**Practicals:**


1. Jeffery, G. H.; Bassett, J.; Mendham, J.; Denney, R. C. (1989), Vogel's Text book of **Quantitative Chemical Analysis**, John Wiley and Sons.
2. Harris, D. C.; Lucy, C. A. (2016), **Quantitative Chemical Analysis**, 9th Edition, Freeman and Company.
3. Day, R. A.; Underwood, A. L. (2012), **Quantitative Analysis**, 6th Edition, PHI Learning Private Limited.


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

## DISCIPLINE SPECIFIC CORE COURSE – 5 (DSC-5): HALOALKANES, ARENES, HALOARENES, ALCOHOLS, PHENOLS, ETHERS AND EPOXIDES

**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 | | |
| Haloalkanes, Arenes, Haloarenes, Alcohols, Phenols, Ethers and Epoxides (DSC-5: Organic Chemistry-II) | 04 | 02 | 0 | 02 | Class 12th Pass | --- |

**Learning Objectives**

The Learning Objectives of this course are as follows:

- To impart understanding of the chemistry of organic functional groups, which include haloalkanes, aromatic hydrocarbons, haloarenes and some oxygen containing functional groups, along with their reactivity patterns.
- To develop understanding of detailed reactions and mechanistic pathways for each functional group to unravel the spectrum of organic chemistry and the extent of organic transformations.
- To aid in the paramount learning of the concepts and their applications.

**Learning outcomes**

**On completion of the course, the student will be able to:**

- Understand reactions of arenes, haloarenes and some oxygen containing functional groups.
- Understand the concept of protection and deprotection
- Use the synthetic chemistry learnt in this course to do functional group transformations.
- Propose plausible mechanisms for the reactions under study.

**SYLLABUS OF DSC-5**

**Unit - 1: Haloalkanes** **( 10 Hours)**

Alkyl halides: Methods of preparation and properties, nucleophilic substitution reactions – $S_N1$, $S_N2$ and $S_Ni$ mechanisms with stereochemical aspects and effect of solvent; nucleophilic substitution v/s elimination.

Organometallic compounds of Mg (Grignard reagent) – Use in synthesis of organic compounds.

**Unit - II: Aromatic Hydrocarbons** **(06 Hours)**

Concept of Aromaticity and anti-aromaticity; Electrophilic aromatic substitution: halogenation, nitration, sulphonation, Friedel Crafts alkylation/acylation with their mechanism. Directing effects of groups in electrophilic substitution.

**Unit - III: Aryl halides** **(04 Hours)**

Preparation (including preparation from diazonium salts) and properties, nucleophilic aromatic substitution; $S_NAr$, Benzyne mechanism. Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

**Unit - IV: Alcohols, Phenols, Ethers & Epoxides** **(10 Hours)**

*Alcohols:* Relative reactivity of 1°, 2°, 3° alcohols, reactions of alcohols with sodium, HX (Lucas test), esterification, oxidation (with PCC, alkaline $KMnO_4$, acidic dichromate, conc. $HNO_3$). Oppenauer oxidation; Diols: oxidation of diols by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement.

*Phenols:* Preparation using Cumene hydroperoxide, Acidity and factors affecting it, Kolbe's–Schmidt reactions, Riemer-Tiemann reaction, Houben–Hoesch condensation, Schotten–Baumann reaction, Fries and Claisen rearrangements and their mechanism.

Ethers and Epoxides: Acid and Base catalyzed cleavage reactions.

**Practical - 60 Hours**

1. Acetylation of any one of the following compounds: amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) and phenols (*β*-naphthol, salicylic acid) by any one method:
   i. Using conventional method ii. Using green approach
2. Benzolyation of one of the following amines (aniline, *o*-, *m*-, *p*-toluidines and *o*, *m*-, *p*-anisidine) or one of the following phenols (*β*-naphthol, resorcinol, *p*-cresol) by Schotten-Baumann reaction.
3. Bromination of acetanilide/aniline/phenol by anyone of the following:
   (a) Green method b) Conventional method
4. Nitration of nitrobenzene/chlorobenzene.
5. Haloform reaction of ethanol.
6. Oxidation of benzyl alcohol to benzoic acid
7. Estimation of the given sample of phenol/amine by:

a) Acetylation b) Bromate-Bromide method

8. Functional group tests for alcohols, phenols, carboxylic acids, phenols, carbonyl compounds, esters.

**Essential/recommended readings**

**Theory:**


1. Morrison, R. N., Boyd, R. N., Bhattacharjee, S.K. (2010), **Organic Chemistry**, 7th Edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
2. Finar, I.L. (2002), **Organic Chemistry**, Volume 1, 6th Edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
3. Ahluwalia, V.K.; Bhagat, P.; Aggarwal, R.; Chandra, R. (2005), **Intermediate for Organic Synthesis,** I.K. International.
4. Solomons, T.W.G., Fryhle, C.B., Snyder, S.A. (2017), **Organic Chemistry**, 12th Edition, Wiley.


**Practical:**


1. Mann, F.G., Saunders, B.C. (2009), **Practical Organic Chemistry**, 4th Edition, Pearson Education.
2. Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (2005), **Vogel's Textbook of Practical Organic Chemistry**, Pearson.
3. Ahluwalia, V.K., Aggarwal, R. (2004), **Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis**, University Press.
4. Ahluwalia, V.K., Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
5. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi
6. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi


**Suggestive readings**


1. Carey, F.A., Sundberg, R. J. (2008), **Advanced Organic Chemistry: Part B: Reaction and Synthesis**, Springer.
2. Bruice, P.Y. (2020), **Organic Chemistry**, 3rd Edition, Pearson.
3. Patrick, G. (2012), **BIOS Instant Notes in Organic Chemistry**, Viva Books.
4. Parashar, R.K., Ahluwalia, V.K. (2018), **Organic Reaction Mechanism,** 4th Edition, Narosa Publishing House.


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

## DISCIPLINE SPECIFIC CORE COURSE – 6 (DSC-6): Thermodynamics and its Applications

**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 Thermodynamics and its Applications (DSC – 6: Physical Chemistry – II) | 04 | 03 | - | 01 | Class XII Pass | ---- |

**Learning Objectives**

The Learning Objectives of this course are as follows:

- To make students understand thermodynamic concepts, terminology, properties of thermodynamic systems, laws of thermodynamics and their correlation with other branches of physical chemistry and make them able to apply thermodynamic concepts to the system of variable compositions, equilibrium and colligative properties.

**Learning outcomes**

On completion of the course, the student will be able to:

- Understand the three laws of thermodynamics, concept of State and Path functions, extensive and intensive properties.
- Derive the expressions of $\Delta U$, $\Delta H$, $\Delta S$, $\Delta G$, $\Delta A$ for an ideal gas under different conditions.
- Explain the concept of partial molar properties.

**SYLLABUS OF DSC-6**

**UNIT – I: Basic Concepts of Chemical Thermodynamics (06 Hours)**

Intensive and extensive variables; state and path functions; isolated, closed and open systems.

Mathematical treatment - Exact and inexact differential, Partial derivatives, Euler's reciprocity rule, cyclic rule.

**UNIT – II: First law and Thermochemistry (15 Hours)**

Concept of heat, Q, work, W, internal energy, U, and statement of first law; enthalpy, H, relation between heat capacities, Joule Thompson Porous Plug experiment, Nature of Joule Thompson coefficient, calculations of Q, W, ΔU and ΔH for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions.

Enthalpy of reactions: standard states; enthalpy of neutralization, enthalpy of hydration, enthalpy of formation and enthalpy of combustion and its applications, bond dissociation energy and bond enthalpy; effect of temperature (Kirchhoff's equations) on enthalpy of reactions.

**UNIT – III: Second Law (15 Hours)**

Concept of entropy; statement of the second law of thermodynamics, Carnot cycle. Calculation of entropy change for reversible and irreversible processes (for ideal gases). Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity (for ideal gases). Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

**UNIT – IV Third Law (03 Hours)**

Statement of third law, unattainability of absolute zero, calculation of absolute entropy of molecules, concept of residual entropy, calculation of absolute entropy of solid, liquid and gases.

**UNIT – V Systems of Variable Composition (06 Hours)**

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs Duhem equation, chemical potential of ideal mixtures, Change in thermodynamic functions on mixing of ideal gases.

**Practical – 30 Hours**

**Thermochemistry:**

(a) Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution of sulphuric acid or enthalpy of neutralization).
(b) Determination of heat capacity of a calorimeter for different volumes using heat gained equal to heat lost by cold water and hot water.
(c) Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

(d) Determination of the enthalpy of ionization of ethanoic acid.
(e) Determination of integral enthalpy solution of endothermic salts.
(f) Determination of integral enthalpy solution of exothermic salts.
(g) Determination of basicity of a diprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
(h) Determination of enthalpy of hydration of salt.
(i) Study of the solubility of benzoic acid in water and determination of ΔH.

Any other experiment carried out in the class.

**Essential/recommended readings**
**Theory**


1. Peter, A.; Paula, J. de. (2011), **Physical Chemistry**, 9th Edition, Oxford University Press.
2. Castellan, G. W. (2004), **Physical Chemistry**, 4th Edition, Narosa.
3. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 2, 6th Edition, McGraw Hill Education.
4. Kapoor, K.L., **A Textbook of Physical Chemistry**, Vol 3, 5th Edition, McGraw Hill Education.
5. McQuarrie, D. A.; Simon, J. D. (2004), **Molecular Thermodynamics**, Viva Books Pvt. Ltd.


**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, McGraw Hill Education.
3. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P. (2003), **Experiments in Physical Chemistry**, 8th Edition, McGraw-Hill, New York.


**Suggestive readings**


1. Levine, I.N. (2010), **Physical Chemistry**, Tata Mc Graw Hill.
2. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A.; Will, S. (2011), **Commonly asked Questions in Thermodynamic**s. CRC Press.


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

# DEPARTMENT OF CHEMISTRY
# Category-I
# B Sc. (Hons) Chemistry

## DISCIPLINE SPECIFIC CORE COURSE -7 (DSC-7): Chemistry of d- and f-block Elements & Quantitative Inorganic Analysis

### 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 | | |
| **Chemistry of d- and f- Elements & quantitative Inorganic Analysis (DSC-7)** | **04** | **02** | **0** | **02** | Passed Class $12^{th}$ with Physics, Chemistry, Mathematics | **NIL** |

### Learning Objectives

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

- To provide thorough knowledge about the d- and f- block elements with respect to the general group trends, physical and chemical properties of these elements.
- To familiarize the students with the d- and f-block elements and get an idea about horizontal similarity in a period in addition to vertical similarity in a group.
- To impart the knowledge about inorganic polymer
- To give an idea about the principles of gravimetric analysis.

### Learning outcomes

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

- List the important properties of transition metals, lanthanoids, and actinoids
- Use Latimer diagrams to predict and identify species which are reducing, oxidizing and tend to disproportionate and calculate skip step potentials.
- Describe the classification, structure and applications of Inorganic Polymers.
- List and use the principles of gravimetric analysis for quantitative analysis

### SYLLABUS OF DSC-7

**UNIT – 1: Transition Elements** **(12 Hours)**

General group trends with special reference to electronic configuration, colour, variable valency, magnetic properties, catalytic properties, and ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer diagrams), Frost diagrams of Mn and Cr.

A brief discussion of differences between the first, second and third transition series

**UNIT – 2: Lanthanoids and Actinoids (8 Hours)**

A brief discussion of electronic configuration, oxidation states, colour, spectral and magnetic properties. Lanthanoid contraction (causes and effects) separation of lanthanoids by ion exchange method.

**UNIT – 3: Inorganic Polymer (8 Hours)**

Comparison with organic polymers, classification, structure and applications of following inorganic polymers:

- Borates
- Silicates, silicones
- Phosphates
- Phosphazenes (for cyclic polymers, only trimer is to be discussed)

**UNIT – 4: Principles of gravimetric analysis (2 Hours)**

Particle size, Precipitation, Coagulation, Peptization, Co-precipitation, Digestion, Filtration and washing the precipitate, Drying and ignition the precipitate

**Practical component (60 Hours)**

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

**(A) Gravimetry**

1. Estimation of Ni(II) using dimethylglyoxime (DMG).
2. Estimation of copper as CuSCN.
3. Estimation of iron as $Fe_2O_3$ by precipitating iron as $Fe(OH)_3$. (by homogeneous and heterogeneous method)
4. Estimation of Al(III) by precipitating with oxime and weighing as $Al(oxime)_3$ (aluminiumoxinate).

**(B) Inorganic Preparations**

1. Potassium aluminium sulphate $KAl(SO_4)_2.12H_2O$ (potash alum) or Potassium chromium sulphate $KCr(SO_4)_2.12H_2O$ (chrome alum).
2. Manganese phosphate and
3. Sodium peroxoborate

**(C ) Paper chromatographic separation of following metal ions (minimum two should be done):**

1. Ni(II) and Co(II)

2. Cu(II) and Cd(II)
3. Fe(III) and Al(III)

**Essential/recommended readings**

**Theory:**


1. Lee, J.D.(2010),**ConciseInorganicChemistry**,WileyIndia.
2. Huheey,J.E.;Keiter,E.A.;Keiter;R.L.;Medhi,O.K.(2009),**InorganicChemistry-PrinciplesofStructureandReactivity**,PearsonEducation.
3. 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.
4. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), **Inorganic Chemistry**, 5th Edition, Pearson.
5. Pfennig, B. W. (2015), **Principles of Inorganic Chemistry**. John Wiley & Sons.
6. Cotton, F.A.; Wilkinson, G. (1999), **Advanced Inorganic Chemistry,** Wiley-VCH.
7. Das, A. K.; Das, M. (2014), **Fundamental Concepts of Inorganic Chemistry**, 1st Edition, Volume 1-3, CBS Publishers & Distributors Pvt. Ltd.
8. Chandrashekhar,V. (2005), **Inorganic and Organometallic Polymers** , 5$^{th}$ Edition, Springer Publications


**Practical:**


1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989), **Vogel's Textbook of Quantitative Chemical Analysis,** John Wiley and Sons,
2. Harris, D. C.; Lucy,C. A.(2016), **Quantitative Chemical Analysis,** 9th Edition, Freeman and Company.
3. Day, R. A.; Underwood, A. L. (2012), **Quantitative Analysis**, Sixth Edition, PHI Learning Private Limited.
4. Marr, G.; Rockett, B.W. (1972), **Practical Inorganic Chemistry**, Van Nostrand Reinhold.


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

## DISCIPLINE SPECIFIC CORE COURSE -8 (DSC-8): Carbonyls, Carboxylic acids, Amines, Nitro compounds, Nitriles, Isonitriles and Diazonium salts

### 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 | | |
| **Carbonyls, Carboxylic Acids, Amines, Nitro Compounds, Nitriles, Isonitriles and Diazonium salts (DSC-8)** | 04 | 03 | 0 | 01 | Passed Class $12^{th}$ with Physics, Chemistry, Mathematics | NIL |

### Learning objectives

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

- To infuse students with the details of the chemistry of aldehydes, ketones, carboxylic acids and their derivatives, nitro, amines and diazonium salts.
- To make students aware of the chemical synthesis, properties, reactions and key applications of the listed classes of compounds and develop understanding of detailed mechanistic pathways for each functional group to unravel the spectrum of organic chemistry and the extent of organic transformations.
- To aid in the paramount learning of the concepts and their applications.

### Learning outcomes

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

- Explain the chemistry of oxygen and nitrogen containing compounds.
- Use the synthetic chemistry learnt in this course to do functional group transformations.
- Propose plausible mechanisms for the reactions under study.

### SYLLABUS OF DSC-8

**UNIT – 1: Carbonyls, Carboxylic acid & their derivatives (27 Hours)**

Carbonyl Compounds: Reaction of carbonyl compounds with ammonia derivatives, Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro and

Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, $\alpha$-substitution reactions, oxidations and reductions (Clemmensen, Wolff Kishner, $LiAlH_4$, $NaBH_4$, MPV, PDC), addition reactions of $\alpha,\beta$-unsaturated carbonyl compounds: Michael addition.
Carboxylic acids and derivatives: Effect of substituents on acidic strength on carboxylic acids, HVZ reaction, typical reactions of dicarboxylic acids and hydroxy acids. Comparative study of nucleophilic acyl substitution for acid chlorides, anhydrides, esters and amides, Mechanism of acidic and alkaline hydrolysis of esters, Dieckmann and Reformatsky reactions, Hoffmann-bromamide degradation and Curtius rearrangement.
Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

**UNIT – 2**: **Nitro Compounds, Amines, Diazonium salts, Nitriles and Isonitriles (18 Hours)**

Nitro compounds: General methods of preparation: from alkyl halides, alkanes, oxidation of amines and oximes. Henry reaction, Nef reaction, Reduction-electrolytic reduction, reaction with nitrous acid, reduction in acidic, basic and neutral medium (for aromatic compounds)

Amines: Preparation**,** chirality in amines (pyramidal inversion), Basicity of amines: Effect of substituents, solvent and steric effects, distinction between Primary, secondary and tertiary amines using Hinsberg's method and nitrous acid, Gabriel Phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction and Cope elimination.

Diazonium Salts**:** Synthetic applications of diazonium salts including preparation of arenes, haloarenes, phenols, cyano and nitro compounds; Coupling reactions of diazonium salts (preparation of azo dyes).

Nitriles: Preparation using following reactions: Dehydration of amides and aldoximes, substitution reaction in alkyl halides and tosylates, from Grignard reagents and from dehydrogenation of primary amines. Properties: Physical properties, discussion on the following reactions with mechanism: Reaction with Grignard reagent, hydrolysis, addition reaction with HX, $NH_3$, reaction with aqueous ROH, Reduction reactions-catalytic reduction and Stephen's reaction, Condensation reactions-Thorpe Nitrile Condensation.

Isonitriles: Preparation from the following reactions: Carbylamine reaction, substitution in alkyl halides and dehydrogenation of N-substituted formamides. Properties: Physical properties, discussion on the following reactions with mechanism: Hydrolysis, reduction, addition of– HX, $X_2$ and sulphur, Grignard reaction, oxidation and rearrangement.

**Practical component (30 Hours)**
**(Laboratory periods:15 classes of 2 hours each)**

1. Preparation of oximes for aldehydes/ketones (like benzaldehyde, ethyl methyl ketone, cyclohexanone etc.)
2. Preparation of semicarbazone derivatives for aldehydes/ketones (like benzaldehyde, ethyl methyl ketone, cyclohexanone etc.)
3. Hydrolysis of amides/esters.
4. Selective reduction of *m*-dinitrobenzene to *m*-nitroaniline.
5. Preparation of S-benzylisothiouronium salts for water soluble and water insoluble carboxylic acids.
6. Systematic qualitative analysis of the given organic compounds containing monofunctional groups (aromatic hydrocarbons, alcohols, phenol) and preparation of one suitable derivative.

Students should be exposed to preparative routes for the synthesis of 3,5-dinitrobenzoate, benzoates, acetate derivatives.

**Note**: The above derivatives should be prepared using 0.5-1.0 g of the organic compound. The solid samples must be collected and may be used for recrystallization, melting point and compound analysis**.**

## Essential/recommended readings

### Theory:


1. Morrison, R. N., Boyd, R. N., Bhattacharjee, S.K. (2010), **Organic Chemistry**, $7^{th}$ Edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
2. Finar, I.L. **Organic Chemistry** Volume 1, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
3. Finar, I.L. **Organic Chemistry** Volume 2, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
4. Solomons, T.W.G., Fryhle, C.B.; Snyder, S.A. (2017), **Organic Chemistry**, $12^{th}$ Edition, Wiley.


### Practical:


1. Vogel, A.I. (2012), **Quantitative Organic Analysis**, Part 3, Pearson Education.
2. Mann, F.G., Saunders, B.C. (2009), **Practical Organic Chemistry**, Pearson Education.
3. Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (2012), **Vogel's Textbook of Practical Organic Chemistry**, $5^{th}$ Edition, Pearson.
4. Ahluwalia, V.K., Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
5. Ahluwalia, V.K., Aggarwal, R. (2004), **Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis**, University Press.
6. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi.
7. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi.

**Suggestive Readings**


1. Mukherji, S.M., Singh, S.P. (2017), **Reaction Mechanism in Organic Chemistry**, Trinity Press.
2. Singh,J., Awasthi, S. K., Singh, Jaya, **Fundamentals of Organic Chemistry-III**, Pragati Prakashan (2023)
3. Carey, F.A., Sundberg, R. J. (2008), **Advanced Organic Chemistry: Part B: Reaction and Synthesis**, Springer.
4. Bruice, P.Y. (2015), **Organic Chemistry,** 3rd Edition, Pearson.
5. Patrick, G. (2003), **BIOS Instant Notes in Organic Chemistry**, Viva Books.


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

# DISCIPLINE SPECIFIC CORE COURSE – 9 (DSC-9): Chemical equilibrium, Ionic equilibrium, conductance and solid state

## 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 equilibrium, Ionic equilibrium, conductance and solid state (DSC-9)** | **04** | **03** | **0** | **01** | **Passed Class XII with Physics, Chemistry and Mathematics** | **NIL** |

### Learning Objectives:

The Learning Objectives of this course are as follows:

- To make students understand the concept of chemical equilibrium and ionic equilibrium.
- To introduce the concept of electrolytes, ionization of various electrolytes, pH.
- To explain the applications of ionization in buffer, hydrolysis, acid-base titrations and indicators.
- To introduce the concept of electrolytic conductance with respect to strong and weak electrolytes and then extend it to understand concepts like ionic mobility, transference and related properties.
- To develop the advance concept of solid state with emphasis on crystal structures in general and cubic crystals in details.

### Learning Outcomes:

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

- Apply the concept of equilibrium to various physical and chemical processes.
- Derive and express the equilibrium constant for various reactions at equilibrium.
- Use Le Chatelier's principle to predict the thermodynamic conditions required to get maximum yield of a reaction
- Apply the concept of equilibrium to various ionic reactions.
- List different types of electrolytes and their properties related to conductance in aqueous solutions.
- Use conductance measurements for calculating many properties of the electrolytes.

- Prepare buffer solutions of appropriate pH.
- Explain the crystal properties and predict the crystal structures of cubic systems form the XRD.
- Use the instruments like pH-meter and conductivity meters.

## SYLLABUS OF DSC-9

**UNIT – 1: Chemical Equilibrium (6 Hours)**

Criteria of thermodynamic equilibrium, degree of advancement of reaction, Chemical equilibria in ideal gases, Thermodynamic derivation of relation between Gibbs free energy of a reaction and reaction quotient, Equilibrium constants and their dependence on temperature, pressure and concentration, Le Chatelier's Principle (Quantitative treatment), Free energy of mixing and spontaneity (qualitative discussion).

**UNIT – 2: Ionic equilibrium (12 Hours)**

Strong, moderate and weak electrolytes, Arrhenius theory of electrolytic dissociation, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono and diprotic acids. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves. Theory of acid–base indicators; selection of indicators and their limitations.

**UNIT – 3: Conductance (12 Hours)**

Quantitative aspects of Faraday's laws of electrolysis, Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch's law of independent migration of ions. Debye-Huckel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rule. Ionic velocity, mobility and their determination, transference number and its relation to ionic mobility, determination of transference number using Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations (v) hydrolysis constants of salts.

**UNIT – 4: Solid state (15 Hours)**

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary idea of symmetry, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl.

## Practical component (30 Hours)
**(Laboratory periods: 15 classes of 2 hours each)**

**pH metry:**
1. Study the effect of addition of HCl/NaOH on pH to the solutions of acetic acid, sodium acetate and their mixtures.
2. Preparation of buffer solutions of different pH values
   a. Sodium acetate-acetic acid
   b. Ammonium chloride-ammonium hydroxide
3. pH metric titration of
   a. Strong acid with strong base
   b. Weak acid with strong base. Determination of dissociation constant of a weak acid.

**Conductometry:**
1. Determination of cell constant
2. Determination of conductivity, molar conductivity, degree of dissociation and dissociation constant of a weak acid.
3. Perform the following conductometric titrations:
   a. Strong acid vs. strong base
   b. Weak acid vs. strong base
   c. Mixture of strong acid and weak acid vs. strong base
   d. Strong acid vs. weak base

**p-XRD** *(p-XRD crystal pattern to be provided to the students)*
1. Differentiate and classify the given set of the diffraction pattern as crystalline materials or amorphous (Glass) substance.
2. Carry out analysis of a given set of p-XRD and determine the type of the cubic crystal structure
   a. NaCl
   b. CsCl
   c. KCl
3. Determination of approximate crystal size from a given set of p-XRD

## Essential/recommended readings
**Theory**


1. Peter, A.; Paula, J. de. (2011), **Physical Chemistry**, 9th Edition, Oxford University Press.
2. Castellan, G. W. (2004), **Physical Chemistry**, 4th Edition, Narosa.
3. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 2, 6th Edition, McGraw Hill Education.
4. McQuarrie, D. A.; Simon, J. D. (2004), **Molecular Thermodynamics**, Viva Books Pvt. Ltd.
5. Kapoor, K.L. (2015),**A Textbook of Physical Chemistry**, Vol 1, 6th 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, McGraw Hill Education.
3. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P. (2003), **Experiments in Physical Chemistry**, 8th Edition, McGraw-Hill, New York.

## Suggestive readings

1. Levine, I.N. (2010), **Physical Chemistry**, Tata Mc Graw Hill.

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

## POOL OF DISCIPLINE SPECIFIC ELECTIVE COURSE

## DISCIPLINE SPECIFIC ELECTIVE COURSE -1 (DSE-1): Nuclear and Environmental 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 | | |
| **Nuclear and Environmental Chemistry (DSE-1)** | **04** | **03** | **0** | **01** | Passed Class 12th with Physics, Chemistry | **NIL** |

### Learning Objectives

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

- To make students know more about nuclear chemistry
- To familiarise the students about environmental chemistry, especially with respect to air and water

### Learning outcomes

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

- Gain knowledge about Nuclear chemistry, radioactive decay, nuclear disasters, and nuclear waste and their disposal.
- Describe the composition of air, various air pollutants, effects and control measures of air pollutants.
- List different sources of water, water quality parameters, impacts of water pollution, water treatment.
- Identify different industrial effluents and their treatment methods.

### SYLLABUS OF DSE-1

**Unit-1 : Nuclear Chemistry** **(21 Hours)**

The nucleus: subatomic particles, e liquid drop model; forces in nucleus-mesons; stability of nucleus-n/p ratio, binding energy; radioactive elements.
Radioactive decay- α-decay, β-decay, γ-decay; neutron emission, positron emission; unit of radioactivity (curie); half life period; radioactive displacement law, radioactive series.
Measurement of radioactivity: ionization chamber, Geiger Counters, Scintillation counters.
Nuclear reactions: Nuclear fission-theory of nuclear fission; chain reaction; nuclear fusion; nuclear reactors-fast breeder reactors, fuels used in nuclear reactors, separation of isotopes, moderators, coolants; nuclear reactors in India.
Applications: Dating of rocks and minerals, carbon dating, neutron activation analysis, isotopic labeling studies, nuclear medicine- $^{99m}Tc$ radio pharmaceuticals.
Nuclear disasters – Chernobyl disaster, Three Mile Island Disaster, Disposal of nuclear waste and its management.

**UNIT – 2: Air Pollution** **(12 Hours)**

Major regions of atmosphere, chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature, Major sources of air pollution, Pollution by $SO_2$, $CO_2$, CO, $NO_x$, $H_2S$ and other foul-smelling gases, methods of estimation of CO, $NO_x$, $SO_x$ and control procedures.

Chemistry and environment impact of the following: Photochemical smog, Greenhouse effect, Ozone depletion

Air pollution control, Settling Chambers, Venturi Scrubbers, Electrostatic Precipitators (ESPs).

**UNIT – 3 : Water Pollution:** **(12 Hours)**

Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological cycle and ecosystems. Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment).

Sludge disposal. Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion-exchange). Water quality parameters for wastewater, industrial water and domestic water.

**Practical component (30 Hours)**
**(Laboratory periods:15 classes of 2 hours each)**
**(At least four experiments to be performed)**

1. Determination of dissolved oxygen in a given sample of water.
2. Determination of Chemical Oxygen Demand (COD) in a given sample of water.
3. Determination of Biological Oxygen Demand (BOD) in a given sample of water.

4. Measurement of chloride, sulphate and salinity of water samples by simple titration method ($AgNO_3$ and potassium chromate).
5. Estimation of total alkalinity of water samples ($CO_3^{2-}$, $HCO_3^-$) using double titration method.
6. Measurement of dissolved $CO_2$ in a given sample of water.
7. Determination of hexavalent Chromium Cr(VI) concentration in tannery wastes/ waste water sample using UV-Vis spectrophotometry technique.

**Essential/recommended readings**

**Theory:**


1. Stanley E. Manahan, 10th edition, **Environmental chemistry,** CRC Press, Taylor and Francis Group, US, 2017
2. Baird, C. and Cann,M., **Environmental Chemistry,**(2012), Fifth Edition, W. H. Freemann & Company, New York, US.
3. VanLoon, G.W. and Duffy, J.S.( 2018) **Environmental Chemistry - A global perspective**, Fourth Edition, Oxford University Press
4. Brusseau, M.L.; Pepper,I.L. and Gerba, C., (2019) **Environmental and Pollution Science**, Third Edition, Academic Press.
5. Masters, G.M., (1974) **Introduction to Environmental Science and Technology**, John Wiley & Sons.
6. Masters, G.M., (2015) **Introduction to Environmental Engineering and Science.** JPrentice Hall India Learning Private Limited.

1. 7.Arnikar, H.J., (1987), Second Edition, **Essentials of Nuclear Chemistry,** Wiley Blackwell Publishers

7. Arnikar, H.J.; Rajurkar, N. S.,(2016) **Nuclear Chemistry through Problems,** New Age International Pvt. Ltd.
8. De, A.K.(2012), **Environmental Chemistry,** New Age International Pvt., Ltd.
9. Khopkar, S.M.(2010), **Environmental Pollution Analysis**, New Age International Publisher.
10. Das, A. K. (2010), ***Fundamentals of Inorganic Chemistry***, Volume 1, Second Edition, CBS Publishers & Distributors Pvt Ltd.
11. Das, A. K. (2012), ***Environment Chemistry with Green chemistry***, Books and Allied (P) Ltd.


**Practical:**


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


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

## DISCIPLINE SPECIFIC ELECTIVE COURSE - 2 (DSE-2): 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 | | |
| **Inorganic Materials of Industrial Importance (DSE-2)** | **04** | **03** | **0** | **01** | Passed Class $12^{th}$ with Physics, Chemistry | **NIL** |

### Learning Objectives

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

- To make students understand the diverse roles of inorganic materials in the industry and to give an insight into how these raw materials are converted into products used in day-to-day life.
- To make students learn about silicates, fertilizers, surface coatings, batteries, engineering materials for mechanical construction.
- To develop the interest of students in the frontier areas of inorganic and material chemistry.

### Learning outcomes

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

- State the composition and applications of the different kinds of glass.
- State the composition of cement and discuss the mechanism of setting of cement.
- Defend the suitability of fertilizers for different kinds of crops and soil.
- Explain the process of formulation of paints and the basic principle behind the protection offered by the surface coatings.
- Describe the principle, working and applications of different batteries.
- Evaluate the synthesis and properties of nano-dimensional materials, various semiconductor and superconductor oxides.

### SYLLABUS OF DSE-2

**Unit 1: Silicate Industries** **( 6 Hours)**

**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.

**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 (6 Hours)**

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

**Unit 3: Surface Coatings (18 Hours)**

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.

**Unit 4: Batteries (9 Hours)**

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

**Unit 5: Nano dimensional materials (6 Hours)**

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

## Practical component (30 Hours)

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

**(At least four experiments to be performed)**

1. Detection of constituents of Ammonium Sulphate fertilizer (Ammonium and Sulphate ions) by qualitative analysis and determine its free acidity.

2. Detection of constituents of CAN fertilizer (Calcium, Ammonium and Nitrate ions) fertilizer and estimation of Calcium content.

3. Detection of constituents of Superphosphate fertilizer (Calcium and Phosphate ions) and estimation of phosphoric acid content.

4. Analysis of (Cu, Ni) in alloy or synthetic samples (methods involving Gravimetry and Spectrophotometry).

5. Analysis of (Cu, Zn) in alloy or synthetic samples (Multiple methods involving Iodometry, and Potentiometry).

6. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.

7. Synthesis of silver nanoparticles by green and chemical approach methods and its characterization using UV-visible spectrophotometer

**Essential/recommended readings**

**Theory:**


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


**Practical:**


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


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

## DISCIPLINE SPECIFIC ELECTIVE COURSE – 3 (DSE-3): Green Chemistry in Organic Synthesis

### 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 | | |
| **Green Chemistry in Organic Synthesis (DSE-3)** | 04 | 03 | 0 | 01 | Passed Class 12th with Physics, Chemistry | Basic knowledge of organic reactions |

### Learning objectives

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

- To create awareness about the chemistry that is not harmful for human health and the environment.
- To provide thorough knowledge of the green chemistry principles that can be used to develop chemistry in greener way.
- To familiarize students with new remediation technologies for the cleaning up of hazardous substances.
- To use green chemistry for boosting profits, increase productivity and ensure sustainability with absolute zero waste.
- To learn about innovations and applications of green chemistry in education that helps companies to gain environmental benefits as well as to achieve economic and societal goals also
- The objective of the practical component is to develop basic skills to be able to design, develop and run chemical processes in a sustainable way.

### Learning outcomes

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

- List the twelve principles of green chemistry and 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
- State the uses of catalyst over stoichiometric reagents
- Debate and use green solvents, renewable feedstock, and renewable energy sources for carrying out safer chemistry
- Use green chemistry for problem solving, innovation and finding solutions to environmental problems.
- Design safer processes, chemicals, and products through understanding of inherently safer design (ISD)

- Discuss the success stories and use real-world cases to practice green chemistry

## SYLLABUS OF DSE-3

**UNIT – 1: Introduction (3 Hours)**

Introduction to Green Chemistry, some important environmental laws, pollution prevention Act of 1990, emergence of green chemistry, need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry. Green chemistry in sustainable development.

**UNIT – 2: Application of Green Chemistry Principles (36 Hours)**

Principles of Green Chemistry and designing a chemical synthesis
Concept familiarization and application of green chemistry principles using specific examples

1. Prevention of waste/ by products; waste or pollution prevention hierarchy
2. Green metrics to assess greenness of a reaction: Calculation of atom economy of the rearrangement, addition, substitution, and elimination reactions; calculation of E-factor for industrial processes
3. Prevention/ minimization of hazardous/ toxic products
4. Safer Solvent and Auxiliaries: Problems associated with conventional reaction media Some Common Green solvents: Introduction, application, advantages, and disadvantages of green solvents in organic synthesis (taking suitable examples). Special emphasis on the following:
   i. Super Critical Fluids (with special reference to carbon dioxide)
   ii. Water: Concept of In-water, and on-water reactions (with special reference to synthesis of terpinol and linalool in water, Benzoin condensation, Heck reaction)
   iii. Ionic Liquids: Physical properties and classification of Ionic Liquids (with special reference to Diels Alder reaction and Coumarin synthesis in ionic liquids)
   iv. Biomass derived Solvents: Physicochemical properties, Use of glycerol and its derivatives (Mizoroki–Heck reaction) and 2-methyltetrahydrofuran (Suzuki–Miyaura reaction).
5. Design for energy efficiency: Phenomenon of accelerating organic reactions by using the following Green Chemistry tools (taking suitable examples) and its advantages:
   i. Mechanochemistry
   ii. Ultrasound assisted reactions: Taking examples like Simmons Smith reaction, Diels–Alder reaction,
   iii. Microwave assisted reactions: Special emphasis on solvent-free synthesis- copper phthalocyanine and aspirin, In-water reactions-Hofmann Elimination, methyl benzoate to benzoic acid and Decarboxylation reaction;
   iv. Electrocatalysis: Taking examples like adiponitrile synthesis, synthesis of 3-bromothiophene.
   v. Visible light induced Reactions: with examples such as, syntheses of caprolactam and vitamin $D_3$, cis-trans isomerization of alkenes
6. Use of renewable starting materials: Illustrate with few examples such as biodiesel, bioethanol, polymers from renewable resources (PLA from corn), Synthesis and properties of 2-Methyltetrahydrofuran, furfural and 5-Aminolevulinic acid (DALA) from levulinic acid

7. Avoidance of unnecessary derivatization – careful use of blocking/protecting groups (taking specific examples like selective oxidation of aldehydic group and synthesis of 6-Aminopenicillanic Acid (6-APA) from penicillin G
8. Catalysis and green chemistry
   Introduction to Catalysis (including concept of selectivity, turnover frequency and turnover number), Types of Catalysts: Heterogeneous catalysis and homogeneous catalysis (H-beta and zeolites in organic synthesis), General catalytic cycle for heterogeneous catalysis; Asymmetric catalysis (Monsanto route to L-dopa via asymmetric hydrogenation, synthesis of carbapenhem via Asymmetric reduction); Photocatalysis (with special reference to $TiO_2$); Biocatalysis (Synthesis of adipic acid/catechol using biocatalyst) and Nanocatalysis (oxazole synthesis using nanocatalyst)
9. Design for degradation: (Illustrate with the help of examples: soaps and detergents, pesticides, polymers)
10. Real Time monitoring of chemical processes using inline, offline, and online techniques
11. Inherently safer design/chemistry:
    Principle and subdivision of ISD, Bhopal Gas Tragedy (safer route to carbaryl) and Flixiborough accident (safer route to cyclohexanol, Asahi Process)

**UNIT – 3: Industrial Applications and Success Stories (6 Hours)**

- Vitamin C Synthesis using enzymes (Hoffman La Roche)
- Zoloft -Presidential Chemistry Award Winning Innovation (Pfizer)
- Methyl Methacrylate syngas process (Eastman Chemicals)
- Synthesis of herbicide disodium iminodiacetate
- Rightfit pigments azo dyes synthesis and their applications
- Healthier Fats and oils by Green Chemistry: Enzymatic Interesterification for production of No Trans-Fats and Oils.
- Synthesis of anti-tuberculosis drug Paramycin from waste water stream

## Practical component (30 Hours) (Laboratory periods:15 classes of 2 hours each)

**Note**: 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 $CO_2$ 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, ethylcyanoacetate 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.
10. Preparation of dibenzalacetone by cross aldol condensation reaction using base catalysed green method.

**Essential/recommended readings**

**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:**


1. Kirchoff, M.; Ryan, M.A. (2002), **Greener approaches to undergraduate chemistry experiment**, American Chemical Society, Washington DC.
2. Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K. (2013), **Green Chemistry Experiments: A monograph**, I.K. International Publishing House Pvt Ltd. New Delhi.
3. Pavia, D.L.; Lamponam, G.H.; Kriz, G.S.W. B. (2012), **Introduction to organic Laboratory Technique- A Microscale approach**, 4th Edition, Brooks-Cole Laboratory Series for Organic chemistry.
4. Sidhwani 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.
5. Sidhwani, I.T; Sharma, R.K. (2020), **An Introductory Text on Green Chemistry**, Wiley India Pvt Ltd.
6. **Monograph on Green Chemistry Laboratory Experiments**, Green Chemistry Task Force Committee, Department of Science and Technology, Government of India.
7. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi
8. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New 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 – 4 (DSE-4): Reactions, Reagents and Chemical Process

### 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 | | |
| **Reactions, Reagents and Chemical Process (DSE-4)** | 04 | 03 | 0 | 01 | Passed Class 12th with Physics, Chemistry | Basic knowledge of organic reactions |

### Learning objectives

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

- To study the important organic name and rearrangement reactions that are crucial for the synthesis of valuable organic compounds.
- To give the knowledge belonging to the role of reagents in organic reactions for the synthesis of chemo-, diastereo- and enantio-selective products.
- To impart the knowledge of process chemistry that is a key part of the large-scale synthesis of chemical products essential for day-to-day life

### Learning outcomes

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

- Explain the reaction mechanism of various name and rearrangement reactions
- Discuss the role of the reagents in organic synthesis and apply these reagents for the bulk chemical synthesis
- Debate and use oxidizing and reducing reagents for selective synthesis organic products
- Apply the learnt techniques to chemical processes
- Acquire skills for human resource building especially in the chemical industry.

### SYLLABUS OF DSE-4

**UNIT – 1: Name Reactions** **(15 Hours)**

Application, scope and mechanism of following reactions: Prevost Reaction, Chugaev Reaction, Maukaiyama Aldol Reaction, Mozingo Reaction, Ramberg Backlund Reaction, Shapiro Reaction, Barbier Reaction, Clark- Eschweiler Reaction, Darzen's Reaction, Julia-Olifination Reaction, Tiffeneaus Damjanov Reaction, Darkin West Reaction, Bischler-Napieralaski Reaction, Birch reduction of aromatic compounds, Appel Reaction, Mitsunobu Reaction, Corey Kim Oxidation, Azide-alkyne 1,3-dipolar cycloaddition reaction, Olefin metathesis: Grubbs reaction, Heck Reaction, Suzuki coupling and Wittig reaction.

**UNIT – 2**: **Reducing Reagents** **(9 Hours)**

Reactions, mechanism and applications of following reducing agents: Sodium borohydride, Lithium aluminium hydride, $NaBH_3CN$, DIBALH, lithium-tri-*tert*-butoxyaluminum hydride, Red-Al $Na[AlH_2(OCH_2OCH_2OCH_3)_2]$, Zinc borohydride, L and K selectrides, $LiBHEt_3$ and $KBHEt_3$, Luche Reagent $NaBH_4$-$CeCl_3$, $K[BH(OAc)_3]$, *bis*-Boric Acid (BBA), Catecholborane, DEMS (Diethoxymethylsilane), 3-Mercapto propionic acid, Polymethylhydrosiloxane (PMHS), Schwartz's Reagent (Zirconocene chloride hydride).

**UNIT – 3: Oxidizing Reagents** **(9 Hours)**

Reactions, mechanism and applications of following oxidizing agents: Jones Reagent ($CrO_3$, $H_2SO_4$, $H_2O$), Swern Reagent (DMSO, oxalyl chloride), Dess Martin, TEMPO, TPAP (Tetrapropyl ammonium perruthenate), Fetizon's Reagent, Fenton's Reagent [$H_2O_2$ + Fe(II) ion], Sodium perborate $NaH_2BO_4$, Sodium Bismuthate $NaBiO_3$, ABNO (9-Azabicyclo[3.3.1]nonane N-oxyl), DEAP (Diethyl allyl phosphate, 

), AZADO (2-Azaadamantane N-oxyl], Wacker oxidation.

**UNIT – 4: Process Chemistry** **(12 Hours)**

1. Process chemistry a) Introduction, stages of scale up process: Bench, pilot, and large-scale process with at least two examples of scale up process of API. b) In-process control and validation of large-scale process.
2. Unit Processes: The following unit processes should be studied with mechanism and one example of each process Nitration: Nitrating agents, process equipment for technical nitration. Halogenation: Types of halogenations, catalytic halogenations. Reduction: Catalytic hydrogenation, hydrogen transfer reactions, metal hydrides. Oxidation: Types of oxidative reactions, and non-metallic oxidizing agents such as H, sodium hypochlorite, oxygen gas, ozonolysis.

## Practical component (30 Hours)

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

1. Oxidation of alcohols to acid using Jones reagent.
2. Reduction of acetophenone and its derivatives to 1-phenyl ethanol derivatives by $NaBH_4$.
3. Reduction of 4-tert-butyl-cyclohexanone to cis and trans 4-tert-butyl-cyclohexanol.
4. Synthesis of 2,5-dimethyl-2,5-hexanediol from tert-butanol using Fenton's reagents.
5. Wittig reaction of benzyltriphenylphosphonium chloride and 4-bromobenzaldehyde using potassium phosphate (tribasic).
6. Substitution ($S_N2$) reaction of 1-iodobutane and 2-naphthol.
7. Aldol condensation reaction: solventless synthesis of chalcones.
9. Borohydride reduction of a ketone: hydrobenzoin from benzil.
10. Visit to chemical industry for the demonstration of pilot scale.

**Essential/recommended readings**

**Theory:**

1. Clayden, J. Greeves, N., Warren, S. **Organic Chemistry**, South Asian Edition, Oxford University Press, USA
2. Gadamasetti K., **Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever- Changing Climate-An Overview**, Vol-2, CRC Press, London.
3. Murphy R.M., **Introduction to Chemical Processes: Principles, Analysis, Synthesis**, McGraw-Hill Education, New York.
4. Harrington P. J., **Pharmaceutical Process Chemistry for Synthesis: Rethinking the Routes to Scale up**, John Wiley and Sons, Inc, New Jersey.
5. Parashar, R.K.; Ahluwalia, V.K. (2018), **Organic Reaction Mechanism,** $4^{th}$ Edition, Narosa Publishing House.
6. Singh J., S. K. Awasthi, Singh Jaya (2023) Fundamental of Organic Chemistry, Paper III, Pragati Prakashan.

**Practical:**

1. Mann F.G, Saunders, B.C., **Practical Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.
2. Vogel A.I., **Elementary Practical Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.

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

## DISCIPLINE SPECIFIC ELECTIVE COURSE -5(DSE-5): Solutions, Colligative properties, Phase Equilibria 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 | | |
| **Solutions, Colligative properties, Phase Equilibria and adsorption (DSE-5)** | **04** | **03** | **0** | **01** | Class $12^{th}$ with Physics, Chemistry | **NIL** |

### Learning Objectives

The Learning Objectives of this course are as follows:

- To make the students understand the various properties of dilute solutions.

- To make the students understand the thermodynamic basis of colligative properties.
- To explain the concept of phase, co-existence of phases, phase diagram for various types of system, CST and distribution law.
- To introduce the concept of adsorption, its dependence on various conditions and applications

## Learning outcomes

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

- Explain different types of phase equilibrium, draw a well labelled phase diagram.
- Predict the existence of a substance in a given phase under different conditions of temperature and pressure
- Apply the concepts of phase, solutions and distribution law while studying other chemistry courses and every-day life processes.
- Explain the type of adsorption that can take place in different systems and predict the conditions to get maximum adsorption.

## SYLLABUS OF DSE-5

**UNIT-1: Solutions and Colligative Properties (12 Hours)**

Dilute solutions; lowering of vapour pressure, Raoult's law, Henry's law. Thermodynamic basis of the colligative properties - lowering of vapour pressure, elevation of Boiling Point, Depression of Freezing point and Osmotic pressure and derivation of expressions for these using chemical potential. Application of colligative properties in calculating molar masses of normal, dissociated and associated solutes in solutions, van't Hoff factor and its applications. Concept of activity and activity coefficients.

**UNIT-2: Phase Equilibria (24 Hours)**

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), with applications. A comparison between the phase diagram of $CO_2$ and $H_2O$. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions (excluding partial miscibility). Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non-ideal), Konovalov's laws, azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications.
Three component systems, water-chloroform-acetic acid system, triangular plots.

**UNIT-3: Surface chemistry (9 Hours)**

Physical adsorption, chemisorption, adsorption isotherms (Langmuir and Freundlich). Nature of adsorbed state. Multilayer adsorption, BET equation derivation, thermodynamic treatment of adsorption-Gibbs equation.

## Practical component (30 Hours)
**(Laboratory periods: 15 classes of 2 hours each)**

**Practical**

**Phase Equilibrium**

1. Determination of critical solution temperature and composition at CST of the phenol water system
2. To study the effect of impurities of sodium chloride and succinic acid on the CST of phenol-water system.
3. To study the cooling curves for the following systems:
   (i) simple eutectic
   (ii) congruently melting systems.

**Adsorption**

Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

## Essential/recommended readings
**Theory:**


1. Peter, A.; Paula, J. de. (2011), **Physical Chemistry**, 9th Edition, Oxford University Press.
2. Castellan, G. W. (2004), **Physical Chemistry**, 4th Edition, Narosa.
3. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 3, 6th Edition, McGraw Hill Education.
4. Kapoor, K.L. (2015),**A Textbook of Physical Chemistry**, Vol 5, 6th Edition, McGraw Hill Education.
5. Ball, D. W. (2017), **Physical Chemistry,** 2nd Edition, Cengage Learning, India.


**Practical:**


4. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), **Senior Practical Physical Chemistry**, R. Chand & Co, New Delhi.
5. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P. (2003), **Experiments in Physical Chemistry**, 8th Edition, McGraw-Hill, New York.


## Suggestive readings


1. Levine, I.N. (2010), **Physical Chemistry**, Tata Mc Graw Hill.


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

## DISCIPLINE SPECIFIC ELECTIVE COURSE- 9 (DSE-9): Applications of Computers 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 | | |
| **Applications of Computers in Chemistry (DSE 9)** | **04** | **03** | **-** | **01** | Class $12^{th}$ with Physics, Chemistry | |

### Learning Objectives

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

- To familiarize the students with the fundamental building blocks and syntax of coding in Python with
- To apply python programming to solve simple Chemistry problems by thinking algorithmically and coding structurally

### Learning outcomes

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

- Understand the importance of python programming in chemistry and its applications in the field of AI and ML
- Perform simple computations in python after learning the basic syntax, loop structure, string data manipulation etc.
- Solve chemistry problems such as finding pKa of a weak acid, solving Schrodinger's equation etc.
- Plot experimental data and perform regression analysis

### SYLLABUS OF DSE-9

**UNIT–1: Basic Computer system** **(Hours: 3)**

Hardware and Software; Input devices, Storage devices, Output devices, Central Processing Unit (Control Unit and Arithmetic Logic Unit); Number system (Binary, Octal and

Hexadecimal Operating System); Computer Codes (BCD and ASCII); Numeric/String constants and variables. Operating Systems (DOS, WINDOWS, and Linux); Software languages: Low level and High-Level languages (Machine language, Assembly language; QBASIC, C, C++, FORTRAN 90&95); Compiled versus interpreted languages. Debugging Software Products (Office, chemsketch, scilab, matlab, and hyperchem), internet application

**UNIT-2: Introduction to Python** **(Hours: 3)**

Why Python? Python coding environment setup, Python as an interpreted language, Brief history of Python, Uses of Python (including artificial intelligence and machine learning), Applications of Python in Chemistry

**UNIT-3: Coding in Python** **(Hours: 18)**

(i) Basic syntax including constants and variables, Operators, Data Types, Declaring and using Numeric data types: int, float, string etc. (ii) Program Flow Control Conditional blocks: if, else and else if, simple FOR loops, FOR loop using ranges, string, list and dictionaries. Use of while loops, Loop manipulation using pass, continue, break and else. (iii) Complex data types: String, List, Arrays, Tuples and Dictionary, String operations and manipulation methods, List operations including slicing, in-built Python Functions. (iv) Python packages - usage of numpy and scipy for mathematical computations.

**UNIT-4: Plotting graphs** **(Hours: 9)**

Matplotlib for Plotting - Simple plots, formatting of plots, multiple plots, histograms, bar graphs, distributions, curve fitting – linear regression.

**UNIT-5: Numerical Methods in Chemistry** **(Hours: 12)**

Solution of quadratic equation, polynomial equations (formula, iteration, Newton – Raphson methods and binary bisection) with examples of polynomial equations used in chemistry; Numerical differentiation – finite difference method (backward, central and forward), Numerical integration - Trapezoidal and Simpson's rule to calculate area under the curves for chemistry problems, e.g., entropy calculations, Simultaneous equations, Statistical analysis- mean, variance, standard deviation, error, Curve fitting – linear regression, Solving Schrödinger's equation using Python packages.

**Practical component**

**Practicals: Python Programming for Chemists** **Credits: 01**

4. **Writing simple programs using scipy and numpy**
    a. syntax, data types
    b. loop structure, conditional loops

c. To learn string data manipulation
d. Array and lists
e. Sorting, matrix manipulations

5. **Plotting graphs using matplotlib**
    a. Planck's distribution law
    b. Maxwell-Boltzmann distribution curves as a function of temperature and mass
    c. Radial distribution curves for hydrogenic orbitals
    d. Gas law Isotherms – Ideal and Real
    e. Data from phase equilibria studies
    f. Wavefunctions and Probabilities as multiplots
    g. Kinetics data with linear fitting

6. **Numerical Methods in Chemistry**
    a. Solving equations involved in chemical equilibria such as pH of a weak acid at a given concentration, cubic equation obtained from solving van der Waals equation of real gases using Iteration, Newton-Raphson, and Binary Bisection Method
    b. Numerical Differentiation – finding equivalence point given pH metric and potentiometric titrations data by finding the first and the second derivative using the finite difference method
    c. Numerical Integration – Trapezoidal and Simpson's 1/3 rule to calculate enthalpy and entropy of an ideal gas
    d. Statistical Analysis – Calculating Mean, Variance, Standard Deviation
    e. Solving Schrodinger's Equation

**Essential/recommended readings**

**Theory:**

7. Dr. M. Kanagasabapathy(2023), **Python for Chemistry: An introduction to Python algorithms, Simulations, and Programing for Chemistry** (English Edition), BPB Publications
8. Robert Johansson (2021), **Numerical Python: Scientific Computing and Data Science Applications with Numpy, SciPy and Matplotlib**, 2nd Edition, Apress

**Practical**

1. Urban M., Murach J., **Murach's Python programming,** $2^{nd}$ Indian reprint 2018, Shroff publishers and distributors
2. Gaddis T., **Starting out with python plus My programming Lab** with Pearson e-text-Access card package, $3^{rd}$ ed.

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

## DEPARTMENT OF CHEMISTRY

## SEMESTER _IV

## B Sc. (Hons) Chemistry

**DISCIPLINE SPECIFIC CORE COURSE - 10(DSC-10): Coordination Chemistry and Reaction Mechanism**

**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 | | |
| Coordination Chemistry and Reaction Mechanism (DSC-10: Inorganic Chemistry - IV) | 04 | 03 | -- | 01 | Class 12th with Physics, Chemistry, Mathematics | -- |

### Learning Objectives

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

- To familiarize the students with coordination compounds which find manifold applications in diverse areas.
- To acquaint the student with the concept of Inorganic reaction mechanism.

### Learning Outcomes

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

- Explain the terms- ligand, denticity of ligands, chelate, coordination number and use standard rules to name coordination compounds.
- Discuss the various types of isomerism possible in such compounds.
- Use Valence Bond Theory to predict the structure and magnetic behaviour of metal complexes and understand the terms inner and outer orbital complexes.

- Explain the meaning of the terms $\Delta_o$, $\Delta_t$, pairing energy, CFSE, high spin and low spin complexes and how CFSE affects thermodynamic properties like lattice enthalpy and hydration enthalpy.
- Explain magnetic properties and colour of complexes on the basis of Crystal Field Theory.
- Explain the reaction mechanism of coordination compounds and differentiate between kinetic and thermodynamic stability.

## SYLLABUS OF DSC-10

**Unit-1: Coordination Chemistry** **(Hours: 28)**

Werner's Coordination theory, simple problems based on this theory

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds (coordination numbers 4 and 6). Valence bond theory and its application to complexes of coordination numbers 4 and 6.

Crystal field theory, measurement of $\Delta_o$. Calculation of CFSE in weak and strong fields, concept of pairing energies, factors affecting the magnitude of $\Delta_o$. Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry: Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory (for octahedral σ-donor, π- acceptor and π- donor complexes).

**Unit-2: Stability of complexes and Inorganic Reaction Mechanism**: **(Hours: 17)**

Brief discussion of thermodynamic and kinetic stability, Factors affecting stability of complexes, such as chelate effect, macrocyclic effect, resonance effect etc., trends in step wise formation constant, interpretation of lability and inertness based on VBT and CFT.

Introduction to inorganic reaction mechanisms, concept of reaction pathways, transition state, intermediate and activated complex. Substitution reactions in square planar complexes, factors affecting the rate of Substitution reactions in square planar complexes- such as charge effect, solvent effect and Trans- effect (Theories of trans-effect).

**Practical component**
**Practical:** **Credits: 01**
**(Laboratory periods: 15 classes of 2 hours each)**

**(A) Argentometry**

Estimation of $Cl^-$

(i) By Mohr's method

(ii) By Vohlard's method and

(iii) By Fajan's method

**(B) Complexometric Titrations:**

(i) Complexometric estimation of $Mg^{2+}$/ $Zn^{2+}$ using EDTA

(ii) Estimation of total hardness of water samples

(iii) Estimation of $Ca^{2+}$ in solution by substitution method

(iv) Estimation of Ca/Mg in drugs or biological samples.

**(C) Properties of Complexes**

Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, dimethyl glyoxime, glycine) by substitution method.

**Essential/recommended readings**

**Theory:**


1. 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.
2. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), **Inorganic Chemistry**, Fifth Edition, Pearson.
3. Huheey, J.E.; Keiter, E.A.; Keiter; R. L.; Medhi, O.K. (2009), **Inorganic Chemistry- Principles of Structure and Reactivity**, Pearson Education.
4. Pfennig, B. W. (2015), **Principles of Inorganic Chemistry,** John Wiley & Sons.
5. Cotton, F.A.; Wilkinson, G.(1999), **Advanced Inorganic Chemistry,** Wiley-VCH.
6. Sodhi G.S. (2018), **Principles of Inorganic Chemistry,** Viva Books India.


**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. Harris, D. C.; Lucy, C. A. (2016), **Quantitative Chemical Analysis,** 9th Edition, Freeman and Company.
3. Day, R. A.; Underwood, A. L. (2012), **Quantitative Analysis**, Sixth Edition, PHI Learning Private Limited.
4. Marr, G.; Rockett, B.W. (1972), **Practical Inorganic Chemistry**, Van Nostrand Reinhold.


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

## DISCIPLINE SPECIFIC CORE COURSE -11 (DSC-11): Carbohydrates, Lipids and Heterocyclic Compounds

### 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 | | |
| Carbohydrates, Lipids and Hetero cyclic Compounds (DSC-11, Organic Chemistry IV) | 04 | 03 | -- | 01 | Class 12$^{th}$ with Physics, Chemistry | -- |

### Learning Objectives

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

- To familiarize students with the chemistry of carbohydrates, lipids, and heterocyclic compounds
- To enable students to develop novel, efficient, convenient, selective and environmentally benign synthetic methods for synthesis of heterocyclic compounds.

### Learning outcomes

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

- Describe uses and applications carbohydrates, lipids and heterocycles
- Use the knowledge gained from study of carbohydrates, lipids and heterocycles to propose greener and better synthetic routes.
- Use the chemistry and biology of carbohydrates, lipids and heterocycles to better serve the mankind.

## SYLLABUS OF DSC-11

**Unit-1: Carbohydrates & Lipids (Hours: 24)**

Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projection and conformational structures; Interconversion of aldoses and ketoses; Killiani-Fischer synthesis and Ruff degradation; Linkage between monosaccharides: Comparative study of the structure of disaccharides (sucrose, maltose, lactose) and polysaccharides (starch, cellulose and glycogen) excluding their structure elucidation. Reactions of disaccharides-reducing property, hydrolysis, methylation and acetylation.
Lipids: Introduction to lipids, classification. Oils and fats: Common fatty acids present in oils and fats, Omega-3&6 fatty acids, trans fats, hydrogenation, hydrolysis, acid value, saponification value, iodine number. Biological importance of triglycerides, phospholipids, glycolipids, and steroids (cholesterol).

**Unit-2: Heterocyclic Compounds (Hours:21)**

Classification and nomenclature of heterocyclic compounds (containing only one hetero atom). Structure, aromaticity in 5-membered and 6-membered rings containing one heteroatom; Basicity and relative reactivity towards electrophilic substitution reactions (amongst five membered and six membered rings.

General methods of synthesis for: furan, thiophene, pyrrole (Paal-Knorr synthesis, Hantzsch synthesis), pyridine (Hantzsch synthesis), indole (Fischer Indole synthesis), quinoline (Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis)

Properties: Physical properties, discussion on the following reaction (with mechanism) for furan, pyrrole, thiophene, pyridine, indole and quinoline: Electrophilic substitution- nitration, sulphonation, halogenation, formylation, acylation, mercuration and carboxylation. Oxidation, reduction, addition, reactions showing acidic /basic character, reaction with diazonium salts, ring opening, ring expansion and nucleophilic substitution reaction wherever applicable should be discussed.

**Practical: Credits: 01**
**(Laboratory periods: 15 classes of 2 hours each)**

1. Estimation of sugars by using Fehling solution.
2. Functional group tests for amine, nitro and amides.
3. Determination of saponification value of the given oil.
4. Determination of iodine number of the given oil.
5. Systematic qualitative analysis of the given organic compounds containing monofunctional groups (carboxylic acids, carbonyl compounds, carbohydrates and esters) and preparation of one suitable derivative.

**Essential/recommended readings**

**Theory:**

1. Berg, J.M., Tymoczko, J.L., Stryer, L. (2019), **Biochemistry**, 9th Edition W.H. Freeman and Co.
2. Nelson, D.L., Cox, M.M., Lehninger, A.L. (2017), **Principles of Biochemistry**. W.H. Freeman and Co., International Edition.
3. Morrison, R. N., Boyd, R. N., Bhattacharjee, S.K. (2010), **Organic Chemistry**, 7th Edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
4. Parashar, R.K., Negi, B. (2016) **Chemistry of Heterocyclic Compounds**, Ane Books Pvt Ltd.
5. Kuashik, S., Singh, A. (2023), **Biomolecules: From Genes to Proteins**, Ist Edition, Berlin, Boston: De Gruyter.
6. Finar, I.L., (2012), **Organic Chemistry** Volume 1, 6th Edition, Pearson Education.
7. Singh J, Awasthi S K, Singh J, **Fundamentals of Organic Chemistry**, Pragati Prakashan Meerut.

**Practical:**

1. Vogel, A.I. (2012), **Quantitative Organic Analysis**, Part 3, Pearson Education.
2. Mann, F.G., Saunders, B.C. (2009), **Practical Organic Chemistry**, Pearson Education.
3. Ahluwalia, V.K., Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
4. Ahluwalia, V.K., Aggarwal, R. (2004), **Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis**, University Press
5. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi
6. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi

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

## DISCIPLINE SPECIFIC CORE COURSE-12 (DSC-12): Electrochemical Cells, Chemical Kinetics and Catalysis

### 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 | | |
| **Electrochemical Cells, Chemical Kinetics and Catalysis (DSC-12, Physical Chemistry IV)** | **04** | **03** | **--** | **01** | **Class $12^{th}$ with Physics, Chemistry, Mathematics** | **--** |

### Learning Objectives

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

- To provide a detailed understanding about galvanic cells and their types
- To explain the applications of galvanic cells and EMF measurements.
- To get an understanding of the kinetics of simple and complex chemical reactions
- To give basic concept about catalysts and enzymes.
- To teach the working of potentiometer and different electrodes for performing potentiometric titrations
- To explain the experimental study of kinetics of simple reactions

### Learning outcomes

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

- Explain the working of electrochemical cells and different types of galvanic cell.
- Devise a spontaneous galvanic cell using various combinations of half-cells.
- Understand the concept of concentration cell
- Use the appropriate galvanic cell to measure pH, calculate thermodynamic parameters and perform potentiometric titrations.
- Write rate law and derive rate equations for simple and complex reactions and understanding of theories of reaction rates.
- Understand different types of catalysts and mechanism of enzyme catalysis.
- Perform potentiometric titrations using appropriate electrodes for quantitative analysis.
- Set up experiments to study the kinetics of simple reactions.

### SYLLABUS OF DSC-12

**Unit-1: Electrochemical Cells (Hours: 21)**

Rules of oxidation/reduction of ions based on half-cell potentials, Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and $SbO/Sb_2O_3$ electrodes. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation). Structure of electric double layer (qualitative aspects only).

**Unit-2: Chemical Kinetics** **(Hours: 18)**

Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods for determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions.

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates, introduction to electrode kinetics (qualitative aspects only).

**Unit-3: Catalysis:** **(Hours: 6)**

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

**Practical:** **Credits: 01**

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

**(A) Potentiometry:**

Perform the following potentiometric titrations:

1. Strong acid vs. strong base
2. Weak acid vs. strong base
3. Dibasic acid vs. strong base
4. Mixture of strong and weak acid vs strong base
5. Potassium dichromate vs. Mohr's salt

**(B) Chemical Kinetics:**

Study the kinetics of the following reactions

1. Iodide-persulphate reaction by Initial rate method
2. Acid hydrolysis of methyl acetate with hydrochloric acid.
3. Saponification of ethyl acetate by conductometric measurements.

**Suggested experiments**

1. To study the kinetics of Iodide-persulphate reaction using integrated rate method.
2. Comparison of the strengths of HCl and $H_2SO_4$ by studying kinetics of hydrolysis of methyl acetate.

**Essential/recommended readings**
**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 3, 6th Edition, McGraw Hill Education.
5. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 5, 3rd Edition, McGraw Hill Education.
6. Laidler K.J. (2003), **Chemical Kinetics**, 3rd Edition, Pearson Education India.


**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, McGraw Hill Education.
3. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P. (2003), **Experiments in Physical Chemistry**, 8th Edition, McGraw-Hill, New York


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

**SEMESTER-V**

**BSC. (HONS.) CHEMISTRY**

## DISCIPLINE SPECIFIC CORE COURSE -13 (DSC-13): Basics of Organometallic 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 | | |
| Basics of Organometallic Chemistry (DSC-13)-Inorganic Chemistry-V | 04 | 03 | -- | 01 | Class 12$^{th}$ with Physics, Chemistry, Mathematics | - |

### Learning Objectives

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

- To familiarize the students with the interactions of metal atom with organic molecules (or not so typical organic molecule), which is in an entirely different fashion as compared to coordination compounds.
- To familiarize the students with the structure and bonding in organometallic compounds
- To familiarize the student with how organometallic compounds can act as good catalysts for organic transformations and hencehave industrial importance associated with medicines, bioorganic synthesis, and energy production.

### Learning Outcomes

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

- Identify and classify organometallic compounds of different types.
- Explain the stability of organometallic compounds and hence the requirement of special experimental conditions for their synthesis.
- Explain the bonding modes through VBT and MOT in these compounds.
- Explain the chemical nature of these compounds through various reactions thus acquiring skills to understand their applications.
- Explain the mechanism of catalysis by these compounds. This may prepare the student to predict the catalytic pathways for new reactions

### SYLLABUS OF DSC-13

**Unit-1: Introduction to Organometallic Chemistry (Hours: 6)**

Definition, brief history, classification of organometallic compounds on the basis of bond type. Common notation used in organometallic chemistry, concept of hapticity of organic ligands, importance of organometallic chemistry, organometallic compounds as reagents, additives, and catalysts. Introduction to the 18-electron rule or effective atomic number rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series and finding metal-metal bonds.

**Unit-2: Structure and Bonding in Organometallic Compounds (Hours : 12)**

Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. Molecular orbital theory applied to organometallic compounds, description of bonding of two electron ligands to transition metals. π-acceptor behavior of CO (MO diagram of CO to be discussed), π-bonding of CO with metal (synergic effect) and use of IR data to explain extent of back bonding, bonding modes of CO, symmetry of metal carbonyls.

Bonding between metal atoms and organic π- systems: linear (ethylene, allyl, butadiene) and cyclic (cyclopentadiene, benzene), Zeise's salt and comparison of synergic effect with that in carbonyls.

Metal alkyls and Metal-carbene complexes

**Unit-3: Synthesis, Reactions and Applications of Organometallic Compounds (Hours: 16)**

General methods of synthesis of metal carbonyls: direct carbonylation, reductive carbonylation, thermal and photochemical decomposition, of mono and binuclear carbonyls of 3d series.

Reaction of metal carbonyls: reduction, oxidation, photochemical substitution, migratory insertion of carbonyls, and nucleophilic addition of CO.

Synthesis of metal-alkene complexes through ligand addition, reduction and substitution and reaction of metal bound alkenes, Zeise's salt

Metal–sandwich compounds**:** Ferrocene: synthesis, physical properties and reactions: acylation, sulfonation, alkylation metallation, acetylation, chloromercuration, Mannich reaction, comparison of aromaticity and reactivity of ferrocene with that of benzene.

Synthesis and reactions of Metal alkyls and Metal-carbenes

**Unit-4: Catalysis by Organometallic Compounds (Hours: 11)**

General principles of catalysis, properties of catalysts, homogeneous and heterogeneous catalysis. (Catalytic steps, examples and industrial applications), deactivation and regeneration of catalysts, (catalytic poisons and promoter).

Organometallic catalysis of the following reactions of commercial importance and their mechanism:

1. Alkene hydrogenation (using Wilkinson's Catalyst)
2. Synthetic gasoline preparation (Fischer Tropsch reaction)
3. Polymerisation of ethene using Ziegler-Natta catalyst
4. Wacker oxidation process (Smidth process)
5. Hydroformylation reaction (Oxo-process)
6. Monsanto Acetic Acid process

**Theoretical aspects of enlisted practicals are also to be included in the theory paper.**

**Practical component**

**Practical: Credits: 01**

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

1. To study and compare the UV-Vis spectrum of ferrocene (in methanol or acetonitrile) and potassium ferrocyanide (in water).
2. To study the cyclic voltammogram of ferrocene.
3. Preparation of Bis(acetylacetonato)copper(II) complex and characterisation through UV-Visible spectrum of its aqueous solution..
4. Preparation of tris(acetylacetonato)manganese(III) complex.
5. Preparation of Potassium tris(oxalato)ferrate(III) complex.
6. Preparation of Tetraamminecopper(II) sulphate monohydrate complex.
7. Preparation of Pentaamminechloridocobalt(III) chloride.
8. Preparation of Hexaamminecobalt(III) chloride
9. Determination of number of chloride ions in ionisation sphere to confirm the formula of complexes prepared in (6) and (7) through potentiometric titration or conductance measurements. (See reference 5 & 6 of Practicals)
10. Compare and interpret the visible spectrum of complexes prepared in (6) and (7) for shifts in wavelength maxima.

**Any other organometallic compounds synthesised from time to time may also be included.**

**Essential/recommended readings**

**Theory:**

1. Gary L Miesler, Paul J Ficsher, and Donald A Tarr, **Inorganic Chemistry** 5$^{th}$ Edition , Pearson.
2. Shriver & Atkins **Inorganic Chemistry,** Edn V, W.H. Freeman and Company.
3. F.A. Cotton & G. Wilkinson, Advanced Inorganic Chemistry, 5th Edition.
4. William W. Porterfield, Inorganic Chemistry, I$^{st}$ Edition.
5. Huheey, J.E.; Keiter, E.A., Keiter; R. L.; Medhi, O.K. (2009), **Inorganic Chemistry-Principles of Structure and Reactivity**, Pearson Education.
6. Principles of Organometallic Chemistry by M.L.H Green, Coward, G.E Coates and K.Wade 3$^{rd}$ Edition.
7. Cotton, F.A.; Wilkinson, G.; Gaus, P.L. **Basic Inorganic Chemistry**, 3$^{rd}$ Edition, Wiley India.
8. Greenwood, N.N.; Earnshaw, A. (1997), **Chemistry of the Elements**, 2$^{nd}$ Edition, Elsevier.
9. Gupta, B. D., Elias, A. J., (2013) **Basic Organometallic Chemistry: Concepts, Syntheses and Applications,** 2$^{nd}$ Edition, Universities Press.

**Practicals:**

1. ChemTexts (2020) 6:22, https://doi.org/10.1007/s40828-020-00119-6
2. J. Chem Education: 1971, Volume 48(2), 133
3. Front. Chem. Sci. Eng. 2013, 7(3): 329–337, DOI 10.1007/s11705-013-1339-0
4. Orbital: Electron. J. Chem. 2019, 11 (6): 348-354

6. Vogel's text book of quantitative chemical analysis. Edn V

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

## DISCIPLINE SPECIFIC CORE COURSE - 14 (DSC-14): Nucleic Acids, Amino Acids, Proteins and Enzymes

### 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 | | |
| **Nucleic Acids, Amino Acids, Proteins and Enzymes (DSC-14, Organic Chemistry- V)** | **04** | **02** | **--** | **02** | Class 12$^{th}$ with Physics, Chemistry | **--** |

### Learning Objectives

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

- To familiarize students with the fascinating chemistry and biology of biomolecules, *i.e.*, nucleic acids and proteins etc..
- To develop the interest of students in the basic concepts of heredity, which are imparted through replication, transcription, and translation processes.
- To discuss basic fundamentals of enzyme action and inhibition, which forms the basis of drug action.

### Learning outcomes

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

- Demonstrate how structure of biomolecules determines their reactivity and biological role.
- Gain insight into concepts of heredity through the study of genetic code, replication, transcription, and translation
- Demonstrate basic understanding of enzyme action and role of inhibitors
- Use knowledge gained to solve real world problems.

### SYLLABUS OF DSC-14

**Unit-1: Nucleic Acids** **(Hours: 8)**

Structure of components of nucleic acids: Bases, Sugars, Nucleosides and Nucleotides. Nomenclature of nucleosides and nucleotides, structure of polynucleotides (DNA and RNA) and factors stabilizing them, biological roles of DNA and RNA; Concept of heredity: Genetic Code, Replication, Transcription and Translation.

**Unit-2: Amino Acids, Peptides and Proteins** **(Hours: 14)**

Amino acids and their classification; α-amino acids - Synthesis, ionic properties, and reactions. zwitterions, pKa values, isoelectric point, and electrophoresis; Study of peptides: determination of their primary structure-end group analysis; Synthesis of peptides using N-protecting, C-protecting and C-activating groups, Solid-phase synthesis; Overview of primary, secondary and tertiary structures of proteins, protein denaturation.

**Unit-3: Enzymes** **(Hours: 8)**

Introduction, classification, and characteristics of enzymes. Salient features of active site of enzymes. Mechanism of enzyme action (taking trypsin as an example), factors affecting enzyme action, coenzymes, and cofactors (including ATP, NAD, FAD), specificity of enzyme action (including stereospecificity). Enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive, and non-competitive inhibition including allosteric inhibition).

**Practical component**
**Practical:** **Credits: 02**
**(Laboratory periods: 15 classes of 4 hours each)**

1. Study of the titration curve of glycine.
2. Estimation of glycine by Sorenson Formol Titration
3. Qualitative analysis of proteins- Ninhydrin test, Biuret test, Millon's reagent test, Xanthoproteic test.
4. Estimation of proteins by Lowry's method.
5. Study of the action of salivary amylase on starch at room temperature.
6. Effect of temperature on the action of salivary amylase.
7. Effect of pH on the action of salivary amylase
8. Study the inhibition of α-Amylase by copper sulphate
9. Isolation and estimation of DNA using cauliflower/onion.

**Essential/recommended readings**

**Theory:**

1. Berg, J.M., Tymoczko, J.L., Stryer, L. (2019), **Biochemistry**, Nineth Edition W.H. Freeman and Co.
2. Nelson, D.L., Cox, M.M., Lehninger, A.L. (2017), **Principles of Biochemistry**. W.H. Freeman and Co., International Edition.
3. Murray, R.K., Granner, D.K., Mayes, P.A., Rodwell, V.W. (2009), **Harper's Illustrated Biochemistry**. Lange Medical Books/McGraw-Hill.
4. Brown, T.A. (2018), **Biochemistry**, (First Indian Edition) Viva Books.
5. Kuashik, S., Singh, A. (2023), **Biomolecules: From Genes to Proteins**, First Edition, Berlin, Boston: De Gruyter.
6. Voet, D., Voet, J.G. (2010), **Biochemistry**, Fourth Edition, Wiley.

7. Singh J, Awasthi S K, Singh J, **Fundamentals of Organic Chemistry**, Pragati Prakashan Meerut.

## Additional Resources:

1. Finar, I.L. (2008), **Organic Chemistry**, Volume 2, Fifth Edition, Pearson Education.
2. Bruice, P.Y. (2020), **Organic Chemistry,** Egighth Edition, Pearson Education.

## Practicals:

1. **Manual of Biochemistry Workshop** (2012), Department of Chemistry, University of Delhi.
2. Kumar, A., Garg, S., Garg, N. (2015), **Biochemical Tests: Principles and Protocols**. Viva Books.
3. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi

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

**DISCIPLINE SPECIFIC CORE COURSE-15 (DSC-15): Quantum Chemistry and Organic Chemistry IV Covalent bonding**

**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 | | |
| **Quantum Chemistry and Covalent bonding (DSC-15, Physical Chemistry V)** | **04** | **03** | **--** | **01** | **Class 12th with Physics, Chemistry, Mathematics** | |

## Learning objectives

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

- To make students understand the limitations of classical mechanics and the need of quantum chemistry
- To familiarize the students with the postulates of quantum chemistry
- To explain how to apply the postulates to derive equations for various models and extend to hydrogen atom and hydrogen like atoms.
- To explain the valence bond and molecular orbital theories and their applications to simple molecules
- To explain the use of some computational software

## Learning outcomes

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

- Explain the limitations of classical mechanics and solution in terms of quantum mechanics for atomic/molecular systems.
- Develop an understanding of quantum mechanical operators, quantization, probability distribution, uncertainty principle
- Set up Schrodinger equations for different types of systems
- Explain the concept of covalent bonding based on valence bond theory and molecular orbital theory.
- Perform calculations using different software and plot different wavefunctions and probability distribution curves.
- Perform simple calculations using appropriate quantum mechanical methods in different computational software

## SYLLABUS OF DSC-15

**Unit-1: Quantum Chemistry** **(Hours: 22)**

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

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

Angular momentum. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation in Cartesian and spherical polar coordinates (derivation not required). Separation of variables. Spherical harmonics. Discussion of solution (Qualitative).

**Unit-2: Hydrogen atom (Hours: 08)**

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part and quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Zeeman effect, Introduction of spin quantum number and magnetic spin quantum number Setting up of Schrödinger equation for many electron atoms (He, Li), Indistinguishability of electrons and Pauli exclusion principle, Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

**Unit-3: Covalent bonding (Hours: 15)**

Setting up of Schrödinger equation, Born-Openheimer approximation, LCAO-MO treatment of $H_2^+$ and its qualitative extension to $H_2$, Valence bond (VB) treatment of $H_2$, Comparison of LCAO-MO and VB wave functions of $H_2$ and their refinements, Qualitative description of LCAO-MO of homonuclear and heteronuclear diatomic molecules-HF and LiH.

**Practical component**

**Practical: Credits: 01**

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

1. Plot the radial wavefunctions and probability distribution for H atom's 1s, 2s, 2p orbital using software like EXCEL.
2. Using a software such as ArgusLab, plot HOMO, LUMO and ESP maps of various molecules.
3. Draw probability plots for a particle in a 1-dimensional box for different values of quantum number n - commenting on the number of points of zero probability and then correlate them with the correspondence principle.
4. Plot the electron density contour maps of sigma molecular orbitals for diatomic homonuclear molecules.
5. Plotting of the wave function and probability curve for simple harmonic motion and interpret the results for first two levels.

6. Plotting energy as a function of distance for simple harmonic motion - parabolic curve.
7. Using software such as ArgusLab calculate properties such as dipole moment and Mulliken charges using quantum mechanical methods.

**Note: Any other suitable software may also be used .**

**Essential/recommended readings**

**Theory:**


1. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, McGraw Hill Education, Vol 4, 5th Edition, McGraw Hill Education.
2. House, J.E. (2004), **Fundamentals of Quantum Chemistry**, 2nd Edition, Elsevier.
3. McQuarrie, D.A. (2016), **Quantum Chemistry**, Viva Books.
4. Chandra, A. K. (2001), **Introductory Quantum Chemistry**, Tata McGraw-Hill.
5. House, J.E. (2004), **Fundamentals of Quantum Chemistry**, 2nd Edition, Elsevier


**Suggested Readings**


1. Atkins, P.W.; Friedman, R. (2010), **Molecular Quantum Mechanics**, 5th Edition, Oxford University Press.


**Practical:**


1. McQuarrie, D. A. **Mathematics for Physical Chemistry** University Science Books (2008).
2. Mortimer, R. **Mathematics for Physical Chemistry**. 3rd Ed. Elsevier (2005).
3. Steiner, E**. The Chemical Maths Book** Oxford University Press (1996).
4. Yates, P. **Chemical Calculations**. 2nd Ed. CRC Press (2007).
5. Levie, R. de, **How to use Excel in analytical chemistry and in general scientific data analysis**, Cambridge Univ. Press (2001) 487 pages.
6. Noggle, J. H. **Physical Chemistry on a Microcomputer**. Little Brown & Co. (1985).


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

## SEMESTER-VI

### BSC. (HONS.) CHEMISTRY

### DISCIPLINE SPECIFIC CORE COURSE -16 (DSC-16): Principles in Qualitative Analysis and Bioinorganic 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 | | |
| **Principles in Qualitative Analysis and Bioinorganic Chemistry (DSC-16: Inorganic Chemistry -VI)** | **04** | **02** | **--** | **02** | Class 12th with Physics, Chemistry, Mathematics | **--** |

### Learning Objectives

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

- To discuss the principles of qualitative analysis
- To understand the concept of solubility products and the common ion effect on the separation of cations.
- To discuss the importance of metal ions in biological systems.
- To discuss the applications of iron in physiology, including iron transport and storage.

### Learning Outcomes:

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

- Explain the basic principles of qualitative inorganic analysis.
- Discuss the influence of solubility products and the common ion effect on the separation of cations.
- Discuss the identification of interfering anions and their removal.
- Explain and discuss the importance of metal ions in biological systems, through discussions on
  metal-containing enzymes, the sodium-potassium pump.
- Discuss the applications of iron in physiology, including iron transport and storage system.

**Unit-1: Theoretical Principles in Qualitative Analysis (Hours: 12)**

Basic principles involved in analysis of cations and anions. Solubility product, common-ion effect. Principles involved in separation of cations into groups and choice of group reagents. Interfering anions (fluoride, borate, oxalate and phosphate), need to remove them after Group II and methods of removal. Analysis of insoluble substances.

**Unit-2: Bioinorganic Chemistry (Hours: 18)**

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / potassium pump, conduction of nerve impulses, Ca-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine, Cisplatin as an anti-cancer drug.

Iron and its application in bio-systems, Haemoglobin, Myoglobin, cytochrome-C-oxidase ; Storage and transfer of iron.

**Practical: Credits: 02**

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

**(A)** Qualitative semi-micro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:
$CO_3^{2-}$, $NO_2^-$, $S^{2-}$, $SO_3^{2-}$, $SO_4^{2-}$, $S_2O_3^{2-}$, $CH_3COO^-$, $F^-$, $Cl^-$, $Br^-$, $I^-$, $NO_3^-$, $BO_3^{3-}$, $C_2O_4^{2-}$, $PO_4^{3-}$, $NH_4^+$, $K^+$, $Pb^{2+}$, $Cu^{2+}$, $Cd^{2+}$, $Bi^{3+}$, $Sn^{2+}$, $Sb^{3+}$, $Fe^{3+}$, $Al^{3+}$, $Cr^{3+}$, $Zn^{2+}$, $Mn^{2+}$, $Co^{2+}$, $Ni^{2+}$, $Ba^{2+}$, $Sr^{2+}$, $Ca^{2+}$, $Mg^{2+}$

**(B)** Mixtures should preferably contain one interfering anion, or insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, $CaF_2$ or $Al_2O_3$) or combination of anions e.g. $CO_3^{2-}$ and $SO_3^{2-}$, $NO_2^-$ and $NO_3^-$, $Cl^-$and $Br^-$, $Cl^-$ and $I^-$, $Br^-$ and $I^-$, $NO_3^-$ and $Br^-$, $NO_3^-$ and $I^-$. Spot tests should be done whenever possible.

**Essential/recommended readings**


1. Svehla, G. (1996), **Vogel's Qualitative Inorganic Analysis**,7th Edition, Prentice Hall.
2. Huheey, J.E.; Keiter, E.A., Keiter; R. L.; Medhi, O. K. (2009), **Inorganic Chemistry Principles of Structure and Reactivity**, Pearson Education.
3. Lippard, S.J.; Berg, J.M. (1994), **Principles of Bioinorganic Chemistry**, Panima Publishing Company.
4. *Biological Inorganic Chemistry* by **RR Crichton** in additional books
5. *Bioinorganic Chemistry- Inorganic Elements in the Chemistry of Life: An Introduction and Guide*, 2nd Edition by **Wolfgang Kaim, Brigitte Schwederski, Alex Klein**
6. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), 5th Edition, Oxford University Press.


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

## DISCIPLINE SPECIFIC CORE COURSE – 17 (DSC-17): Polynuclear Hydrocarbons, Photochemistry, Pericyclic Reactions, and Spectroscopy of Organic Compounds

### 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 | | |
| **Polynuclear Hydrocarbons, Photochemistry, Pericyclic Reactions, and Spectroscopy of Organic Compounds (DSC-17, Organic Chemistry-VI)** | 04 | 03 | -- | 01 | Class 12th with Physics, Chemistry | - |

## Learning objectives

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

- To provide thorough knowledge of the chemistry of polynuclear hydrocarbons .
- To detail the basic principles and applications of pericyclic reactions and photochemistry
- To familiarize students with the various tools and techniques for identifying and characterizing the organic compounds through their interactions with electromagnetic radiations *viz.* UV-Visible, IR and NMR spectroscopy.

## Learning outcomes

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

- Discuss and use the chemistry of polynuclear hydrocarbons for application in real world problems.
- Discuss and use the pericyclic reactions and photochemistry for research and other applications.
- Use spectroscopic techniques to determine structure and stereochemistry of known and unknown compounds.

## SYLLABUS OF DSC-17

**Unit-1: Polynuclear Hydrocarbons** **(Hours: 6)**

Introduction, classification, structure, nomenclature and uses. Aromaticity of polynuclear hydrocarbons, structure elucidation of Naphthalene and general methods of preparation of naphthalene and anthracene (including Haworth method, Friedel Craft acylation, Diels Alder reaction, Elbs reaction). Relative reactivity of naphthalene and anthracene in comparison to benzene.

Discussion on the following reactions (with mechanism) for Naphthalene and Anthracene: Addition reactions, Oxidation, Electrophilic substitution- Friedel Craft reaction, Chloromethylation, Halogenation, Formylation, Nitration and sulphonation. Reduction reaction and Diels Alder reaction.

**Unit-2**: **Photochemistry and Pericyclic reactions** **(Hours: 12)**

**Photochemistry**

Introduction and basic principles of photochemistry, photochemical energy, photolytic cleavage, photochemistry of carbonyl compounds (Norrish type 1, Norrish type 2 and Peterno Buchi reactions)

**Pericyclic Reactions**

Introduction: Types of pericyclic reactions (Electrocyclic, Cycloaddition and Sigmatropic Rearrangements), Symmetry in σ and π molecular orbitals, Frontier Molecular Orbitals.

Electrocyclic Reactions: Conrotatory and Disrotatory motion in ring opening and ring closing reactions in (4n) and (4n+2) π electron systems, FMO method, Woodward Hoffmann rule.

Cycloaddition Reactions: [2+2] and [4+2] π cycloaddition reactions, Diels Alder reaction (electron rich and electron poor dienes and dienophiles, Stereochemistry, Alder rule of endo addition).

Sigmatropic Reactions: [1,3], [1,5] and [3,3] sigmatropic rearrangements, Cope rearrangement, Claisen Rearrangements.

**Unit-3**: **Spectroscopy of Organic Compounds (Hours: 27)**

UV-Visible Spectroscopy: Types of electronic transitions, $\lambda_{max}$, chromophores and Auxochromes, bathochromic and hypsochromic shifts, intensity of absorption, factors affecting $\lambda_{max}$ values, application of Woodward Rules for calculation of $\lambda_{max}$ for the following systems: $\alpha$, $\beta$-unsaturated aldehydes, ketones, carboxylic acids and esters; conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between *cis* and *trans* isomers by UV; Colour concept, Theory of colour and constitution-Witt's theory, valence bond and molecular orbital theory.

IR Spectroscopy: Fundamental and non-fundamental molecular vibrations; IR absorption positions of O and N containing functional groups; effect of H-bonding, conjugation, resonance and ring size on IR absorptions; fingerprint region and its significance, application of IR in functional group analysis.

$^1$H-NMR Spectroscopy: Basic principles of proton magnetic resonance, chemical shift and factors, influencing it; equivalent and non-equivalent protons (chemical and magnetic equivalence), Spin–Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics. Interpretation of NMR spectra of simple compounds containing AX, $AX_2$, $AX_3$, $A_2X_3$ spin systems, special case of 1-nitropropane.

Applications of IR, UV and $^1$H-NMR Spectroscopy for identification of simple organic compounds (spectra to be provided for some representative compounds).

**Practical component**

**Practical: Credits: 01**

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

1. Systematic qualitative analysis of the given organic compounds containing monofunctional groups (Aryl halides, nitro compounds, amines and amides) and simple

bifunctional compounds like salicylic acid, cinnamic acid, *p*-nitro phenol etc. and preparation of one suitable crystalline derivative.

2. Differentiation between of *o*-/*p*-hydroxybenzaldehyde by IR spectroscopy (Spectra to be provided).
3. Differentiation between of benzoic acid and cinnamic acid by UV spectroscopy (Spectra to be provided).

**Essential/recommended readings**

## Theory:


1. Morrison, R. N., Boyd, R. N., Bhattacharjee, S.K. (2010), **Organic Chemistry**, 7th Edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
2. Finar, I.L. **Organic Chemistry** Volume 1, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
3. Finar, I.L. **Organic Chemistry** Volume 2, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
4. Solomons, T.W.G., Fryhle, C.B.; Snyder, S.A. (2017), **Organic Chemistry**, 12th Edition, Wiley.
5. Silverstein R.M. (2005), **Spectrometric Identification of organic compounds**, 7th edition, John Wiley and Sons,
6. Kemp W. (2019), **Organic Spectroscopy**, Third Edition, MacMillan.
7. Pavia, D. (2015), **Introduction to Spectroscopy**, Fifth Edition, Cengage Learning India Pvt. Learning.
8. Scheinmann, F., **Introduction to spectroscopic methods for identification of organic compounds**, Volume 2, Pergamon Press.
9. Ahluwalia, V.K., Parashar, R.K. (2011), **Organic Reaction Mechanisms**, 4th Edition, Narosa Publishing House.
10. Horspool, W.M. (1976) **Aspects of Organic Photochemistry**, Academic Press.
11. Singh J, Awasthi S K, Singh J, **Fundamentals of Organic Chemistry**, Pragati Prakashan Meerut.


## Practical:


1. Vogel, A.I. (2012), **Quantitative Organic Analysis**, Part 3, Pearson Education.
2. Mann, F.G., Saunders, B.C. (2009), **Practical Organic Chemistry**, Pearson Education.
3. Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (2012), **Vogel's Textbook of Practical Organic Chemistry**, Fifth Edition, Pearson.
4. Ahluwalia, V.K., Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
5. Ahluwalia, V.K., Aggarwal, R. (2004), **Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis**, University Press
6. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi
7. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi

## DISCIPLINE SPECIFIC CORE COURSE-18 (DSC-18): Photochemistry 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 | | |
| **Photochemistry and Spectroscopy (DSC-18, Physical Chemistry VI)** | **04** | **02** | **-** | **02** | **Class XII with Physics, Chemistry and Mathematics** | |

### Learning Objectives:

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

- To make students understand the laws of photochemistry and their applications
- To understand the basis of molecular spectroscopy
- To study different types of spectroscopic techniques and their applications

### Learning Outcomes:

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

- Explain low and high quantum yield
- Explain photosensitized reactions
- Apply the concept of quantization to spectroscopy.
- Interpret various types of spectra and know about their application in structure elucidation

### SYLLABUS OF DSC-18

**Unit-1: Introduction to Molecular Spectroscopy and Photochemistry (Hours: 6)**

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

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

**Unit-2: Rotational, Vibrational , Raman and Electronic Spectroscopy (Hours: 14)**

**Rotational spectroscopy**: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic molecules, isotopic substitution, classification of molecules based on moment of inertia, applications of rotation spectroscopy (e.g. microwave appliances)

**Vibrational spectroscopy**: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies.

Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

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

**Electronic spectroscopy**

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

**Unit-3: NMR and ESR (Hours: 10)**

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

Principles of ESR spectroscopy, hyperfine structures, ESR of simple radicals

**Practical component**

**Practical: Credits: 02**

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

**(A) Colorimetry :**

1. Verify Lambert-Beer's law and determine the concentration of (i) $CuSO_4$ (ii) $KMnO_4$ (iii) $K_2Cr_2O_7$ in a solution of unknown concentration

2. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$in a mixture.
3. Study the kinetics of iodination of propanone in acidic medium.
4. Determine the amount of iron present in a sample using 1,10-phenathroline.
5. Determine the dissociation constant of an indicator (phenolphthalein).
6. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide

**(B) UV/Visible spectroscopy**:

1. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M $H_2SO_4$) and determine the $\lambda_{max}$ values. Calculate the energies of the two transitions in different units (J molecule$^{-1}$, kJ mol$^{-1}$, cm$^{-1}$, eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2- propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

**(C) Analysis of the given vibration-rotation spectrum of HCl(g)**

**Essential/recommended readings**

**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, 5th Edition, McGraw Hill Education.
3. Kakkar, R. (2015), **Atomic & Molecular Spectroscopy**, Cambridge University Press.

**Suggested Readings:**

1. Engel, T.; Reid, P. (2013), **Quantum Chemistry and Spectroscopy**, Pearson

**Practical:**

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

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

POOL OF DSE FOR III/IV/V/VI SEMESTER

# DISCIPLINE SPECIFIC ELECTIVE COURSE - 1 (DSE-1): 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 | | |
| **Inorganic Materials of Industrial Importance (DSE-1)** | **04** | **03** | **--** | **01** | Class 12th with Physics, Chemistry | **--** |

## Learning Objectives

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

- To make students understand the diverse roles of inorganic materials in the industry and to give an insight into how these raw materials are converted into products used in day-to-day life.
- To make students learn about silicates, fertilizers, surface coatings, batteries, engineering materials for mechanical construction.
- To develop the interest of students in the frontier areas of inorganic and material chemistry.

## Learning outcomes

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

- State the composition and applications of the different kinds of glass.
- State the composition of cement and discuss the mechanism of setting of cement.
- Defend the suitability of fertilizers for different kinds of crops and soil.
- Explain the process of formulation of paints and the basic principle behind the protection offered by the surface coatings.
- Describe the principle, working and applications of different batteries.
- Evaluate the synthesis and properties of nano-dimensional materials, various semiconductor and superconductor oxides.

## SYLLABUS OF DSE-1

**Unit 1: Silicate Industries** **( 6 Hours**

**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.

**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 ( 6 Hours)**

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

**Unit 3: Surface Coatings ( 18 Hours**

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.

**Unit 4: Batteries (9 Hours)**

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

**Unit 5: Nano dimensional materials (6 Hours)**

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

**Practical component**

**Practicals: Credits:**

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

**(At least four experiments to be performed)**

1. Detection of constituents of Ammonium Sulphate fertilizer (Ammonium and Sulphate ions) by qualitative analysis and determine its free acidity.

2. Detection of constituents of CAN fertilizer (Calcium, Ammonium and Nitrate ions) fertilizer and estimation of Calcium content.

3. Detection of constituents of Superphosphate fertilizer (Calcium and Phosphate ions) and estimation of phosphoric acid content.

4. Analysis of (Cu, Ni) in alloy or synthetic samples (methods involving Gravimetry and Spectrophotometry).

5. Analysis of (Cu, Zn) in alloy or synthetic samples (Multiple methods involving Iodometry, and Potentiometry).

6. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.

7. Synthesis of silver nanoparticles by green and chemical approach methods and its characterization using UV-visible spectrophotometer

**Essential/recommended readings**

**Theory:**


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


**Practical:**


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


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

## DISCIPLINE SPECIFIC ELECTIVE COURSE – 2 (DSE-2): Green Chemistry in Organic Synthesis

### 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 | | |
| **Green Chemistry in Organic Synthesis (DSE-2)** | 04 | 03 | -- | 01 | Class 12th with Physics, Chemistry | Basic knowledge of organic reactions |

### Learning objectives

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

- To create awareness about the chemistry that is not harmful for human health and the environment.
- To provide thorough knowledge of the green chemistry principles that can be used to develop chemistry in greener way.
- To familiarize students with new remediation technologies for the cleaning up of hazardous substances.
- To use green chemistry for boosting profits, increase productivity and ensure sustainability with absolute zero waste.
- To learn about innovations and applications of green chemistry in education that helps companies to gain environmental benefits as well as to achieve economic and societal goals also
- The objective of the practical component is to develop basic skills to be able to design, develop and run chemical processes in a sustainable way.

### Learning outcomes

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

- List the twelve principles of green chemistry and 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
- State the uses of catalyst over stoichiometric reagents
- Debate and use green solvents, renewable feedstock, and renewable energy sources for carrying out safer chemistry
- Use green chemistry for problem solving, innovation and finding solutions to environmental problems.

- Design safer processes, chemicals, and products through understanding of inherently safer design (ISD)
- Discuss the success stories and use real-world cases to practice green chemistry

## SYLLABUS OF DSE-2

**UNIT – 1: Introduction (3 Hours**

Introduction to Green Chemistry, some important environmental laws, pollution prevention Act of 1990, emergence of green chemistry, need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry. Green chemistry in sustainable development.

**UNIT – 2: Application of Green Chemistry Principles (36 Hours**

Principles of Green Chemistry and designing a chemical synthesis
Concept familiarization and application of green chemistry principles using specific examples

1. Prevention of waste/ by products; waste or pollution prevention hierarchy
2. Green metrics to assess greenness of a reaction: Calculation of atom economy of the rearrangement, addition, substitution, and elimination reactions; calculation of E-factor for industrial processes
3. Prevention/ minimization of hazardous/ toxic products
4. Safer Solvent and Auxiliaries: Problems associated with conventional reaction media Some Common Green solvents: Introduction, application, advantages, and disadvantages of green solvents in organic synthesis (taking suitable examples). Special emphasis on the following:
   i. Super Critical Fluids (with special reference to carbon dioxide)
   ii. Water: Concept of In-water, and on-water reactions (with special reference to synthesis of terpinol and linalool in water, Benzoin condensation, Heck reaction)
   iii. Ionic Liquids: Physical properties and classification of Ionic Liquids (with special reference to Diels Alder reaction and Coumarin synthesis in ionic liquids)
   iv. Biomass derived Solvents: Physicochemical properties, Use of glycerol and its derivatives (Mizoroki–Heck reaction) and 2-methyltetrahydrofuran (Suzuki–Miyaura reaction).
5. Design for energy efficiency: Phenomenon of accelerating organic reactions by using the following Green Chemistry tools (taking suitable examples) and its advantages:
   i. Mechanochemistry
   ii. Ultrasound assisted reactions: Taking examples like Simmons Smith reaction, Diels–Alder reaction,
   iii. Microwave assisted reactions: Special emphasis on solvent-free synthesis- copper phthalocyanine and aspirin, In-water reactions-Hofmann Elimination, methyl benzoate to benzoic acid and Decarboxylation reaction;
   iv. Electrocatalysis: Taking examples like adiponitrile synthesis, synthesis of 3-bromothiophene.
   v. Visible light induced Reactions: with examples such as, syntheses of caprolactam and vitamin $D_3$, cis-trans isomerization of alkenes
6. Use of renewable starting materials: Illustrate with few examples such as biodiesel, bioethanol, polymers from renewable resources (PLA from corn), Synthesis and

properties of 2-Methyltetrahydrofuran, furfural and 5-Aminolevulinic acid (DALA) from levulinic acid

7. Avoidance of unnecessary derivatization – careful use of blocking/protecting groups (taking specific examples like selective oxidation of aldehydic group and synthesis of 6-Aminopenicillanic Acid (6-APA) from penicillin G
8. Catalysis and green chemistry
   Introduction to Catalysis (including concept of selectivity, turnover frequency and turnover number), Types of Catalysts: Heterogeneous catalysis and homogeneous catalysis (H-beta and zeolites in organic synthesis), General catalytic cycle for heterogeneous catalysis; Asymmetric catalysis (Monsanto route to L-dopa via asymmetric hydrogenation, synthesis of carbapenhem via Asymmetric reduction); Photocatalysis (with special reference to $TiO_2$); Biocatalysis (Synthesis of adipic acid/catechol using biocatalyst) and Nanocatalysis (oxazole synthesis using nanocatalyst)
9. Design for degradation: (Illustrate with the help of examples: soaps and detergents, pesticides, polymers)
10. Real Time monitoring of chemical processes using inline, offline, and online techniques
11. Inherently safer design/chemistry:
    Principle and subdivision of ISD, Bhopal Gas Tragedy (safer route to carbaryl) and Flixiborough accident (safer route to cyclohexanol, Asahi Process)

**UNIT – 3: Industrial Applications and Success Stories (6 Hours)**

- Vitamin C Synthesis using enzymes (Hoffman La Roche)
- Zoloft -Presidential Chemistry Award Winning Innovation (Pfizer)
- Methyl Methacrylate syngas process (Eastman Chemicals)
- Synthesis of herbicide disodium iminodiacetate
- Rightfit pigments azo dyes synthesis and their applications
- Healthier Fats and oils by Green Chemistry: Enzymatic Interesterification for production of No Trans-Fats and Oils.
- Synthesis of anti-tuberculosis drug Paramycin from waste water stream

## Practical component Credits:

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

**Note**: 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 $CO_2$ 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, ethylcyanoacetate 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.
10. Preparation of dibenzalacetone by cross aldol condensation reaction using base catalysed green method.

**Essential/recommended readings**

**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:**

1. Kirchoff, M.; Ryan, M.A. (2002), **Greener approaches to undergraduate chemistry experiment**, American Chemical Society, Washington DC.
2. Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K. (2013), **Green Chemistry Experiments: A monograph**, I.K. International Publishing House Pvt Ltd. New Delhi.
3. Pavia, D.L.; Lamponam, G.H.; Kriz, G.S.W. B. (2012), **Introduction to organic Laboratory Technique- A Microscale approach**, 4th Edition, Brooks-Cole Laboratory Series for Organic chemistry.
4. Sidhwani 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.
5. Sidhwani, I.T; Sharma, R.K. (2020), **An Introductory Text on Green Chemistry**, Wiley India Pvt Ltd.
6. **Monograph on Green Chemistry Laboratory Experiments**, Green Chemistry Task Force Committee, Department of Science and Technology, Government of India.
7. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi
8. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi

## DISCIPLINE SPECIFIC ELECTIVE COURSE -3(DSE-3): Solutions, Colligative properties, Phase Equilibria 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 | | |
| **Solutions, Colligative properties, Phase Equilibria and adsorption (DSE-3)** | **04** | **03** | **-** | **01** | Class 12th with Physics, Chemistry | |

### Learning Objectives

The Learning Objectives of this course are as follows:

- To make the students understand the various properties of dilute solutions.
- To make the students understand the thermodynamic basis of colligative properties.
- To explain the concept of phase, co-existence of phases, phase diagram for various types of system, CST and distribution law.
- To introduce the concept of adsorption, its dependence on various conditions and applications

### Learning outcomes

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

- Explain different types of phase equilibrium, draw a well labelled phase diagram.
- Predict the existence of a substance in a given phase under different conditions of temperature and pressure
- Apply the concepts of phase, solutions and distribution law while studying other chemistry courses and every-day life processes.
- Explain the type of adsorption that can take place in different systems and predict the conditions to get maximum adsorption.

### SYLLABUS OF DSE-3

**UNIT-1: Solutions and Colligative Properties** **(12 Hours**

Dilute solutions; lowering of vapour pressure, Raoult's law, Henry's law. Thermodynamic basis of the colligative properties - lowering of vapour pressure, elevation of Boiling Point, Depression of Freezing point and Osmotic pressure and derivation of expressions for these using chemical potential. Application of colligative properties in calculating molar masses of normal, dissociated and associated solutes in solutions, van't Hoff factor and its applications. Concept of activity and activity coefficients.

**UNIT-2: Phase Equilibria** **(24 Hours)**

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), with applications. A comparison between the phase diagram of $CO_2$ and $H_2O$. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions (excluding partial miscibility). Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non-ideal), Konovalov's laws, azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications.
Three component systems, water-chloroform-acetic acid system, triangular plots.

**UNIT-3: Surface chemistry** **(9 Hours**

Physical adsorption, chemisorption, adsorption isotherms (Langmuir and Freundlich). Nature of adsorbed state. Multilayer adsorption, BET equation derivation, thermodynamic treatment of adsorption-Gibbs equation.

**Practical component** **Credit: 01**
**(Laboratory periods: 15 classes of 2 hours each)**

**Practical**

**Phase Equilibrium**

1. Determination of critical solution temperature and composition at CST of the phenol water system
2. To study the effect of impurities of sodium chloride and succinic acid on the CST of phenol-water system.
3. To study the cooling curves for the following systems:
   (i) simple eutectic
   (ii) congruently melting systems.

**Adsorption**

Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

**Essential/recommended readings**

**Theory:**

1. Peter, A.; Paula, J. de. (2011), **Physical Chemistry**, 9$^{th}$ Edition, Oxford University Press.
2. Castellan, G. W. (2004), **Physical Chemistry**, 4$^{th}$ Edition, Narosa.
3. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 3, 6$^{th}$ Edition, McGraw Hill Education.
4. Kapoor, K.L. (2015),**A Textbook of Physical Chemistry**, Vol 5, 6th Edition, McGraw Hill Education.
5. Ball, D. W. (2017), **Physical Chemistry,** 2$^{nd}$ Edition, Cengage Learning, India.

**Practical:**

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), **Senior Practical Physical Chemistry**, R. Chand & Co, New Delhi.
2. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P. (2003), **Experiments in Physical Chemistry**, 8$^{th}$ Edition, McGraw-Hill, New York.

## Suggestive readings

1. Levine, I.N. (2010), **Physical Chemistry**, Tata Mc Graw Hill.

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

## DISCIPLINE SPECIFIC ELECTIVE COURSE -4 (DSE-4): Nuclear and Environmental 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 | | |
| **Nuclear and Environmental Chemistry (DSE-4)** | **04** | **03** | **--** | **01** | Class 12th with Physics, Chemistry | **--** |

### Learning Objectives

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

- To make students know more about nuclear chemistry
- To familiarise the students about environmental chemistry, especially with respect to air and water

### Learning outcomes

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

- Gain knowledge about Nuclear chemistry, radioactive decay, nuclear disasters, and nuclear waste and their disposal.
- Describe the composition of air, various air pollutants, effects and control measures of air pollutants.
- List different sources of water, water quality parameters, impacts of water pollution, water treatment.
- Identify different industrial effluents and their treatment methods.

### SYLLABUS OF DSE-4

**Unit-1 : Nuclear Chemistry** **(21 Hours**

The nucleus: subatomic particles, e liquid drop model; forces in nucleus-mesons; stability of nucleus-n/p ratio, binding energy; radioactive elements.
Radioactive decay- α-decay, β-decay, γ-decay; neutron emission, positron emission; unit of radioactivity (curie); half life period; radioactive displacement law, radioactive series.
Measurement of radioactivity: ionization chamber, Geiger Counters, Scintillation counters.
Nuclear reactions: Nuclear fission-theory of nuclear fission; chain reaction; nuclear fusion; nuclear reactors-fast breeder reactors, fuels used in nuclear reactors, separation of isotopes, moderators, coolants; nuclear reactors in India.
Applications: Dating of rocks and minerals, carbon dating, neutron activation analysis, isotopic labeling studies, nuclear medicine- $^{99m}Tc$ radio pharmaceuticals.
Nuclear disasters – Chernobyl disaster, Three Mile Island Disaster, Disposal of nuclear waste and its management.

**UNIT – 2: Air Pollution** **(**12 Hours

Major regions of atmosphere, chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature, Major sources of air pollution, Pollution by $SO_2$, $CO_2$, CO, $NO_x$, $H_2S$ and other foul-smelling gases, methods of estimation of CO, $NO_x$, $SO_x$ and control procedures.

Chemistry and environment impact of the following: Photochemical smog, Greenhouse effect, Ozone depletion

Air pollution control, Settling Chambers, Venturi Scrubbers, Electrostatic Precipitators (ESPs).

**UNIT – 3 : Water Pollution:** **(12 Hours)**

Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological cycle and ecosystems. Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment).

Sludge disposal. Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion-exchange). Water quality parameters for wastewater, industrial water and domestic water.

**Practical component**
**Practical:** **Credits: 01**
**(Laboratory periods:15 classes of 2 hours each)**
**(At least four experiments to be performed)**

1. Determination of dissolved oxygen in a given sample of water.
2. Determination of Chemical Oxygen Demand (COD) in a given sample of water.
3. Determination of Biological Oxygen Demand (BOD) in a given sample of water.

4. Measurement of chloride, sulphate and salinity of water samples by simple titration method ($AgNO_3$ and potassium chromate).
5. Estimation of total alkalinity of water samples ($CO_3^{2-}$, $HCO_3^-$) using double titration method.
6. Measurement of dissolved $CO_2$ in a given sample of water.
7. Determination of hexavalent Chromium Cr(VI) concentration in tannery wastes/ waste water sample using UV-Vis spectrophotometry technique.

**Essential/recommended readings**

**Theory:**


1. Stanley E. Manahan, 10th edition, **Environmental chemistry,** CRC Press, Taylor and Francis Group, US, 2017
2. Baird, C. and Cann, M., **Environmental Chemistry,**(2012), Fifth Edition, W. H. Freemann & Company, New York, US.
3. VanLoon, G.W. and Duffy, J.S.( 2018) **Environmental Chemistry - A global perspective**, Fourth Edition, Oxford University Press
4. Brusseau, M.L.; Pepper,I.L. and Gerba, C., (2019) **Environmental and Pollution Science**, Third Edition, Academic Press.
5. Masters, G.M., (1974) **Introduction to Environmental Science and Technology**, John Wiley & Sons.
6. Masters, G.M., (2015) **Introduction to Environmental Engineering and Science.** JPrentice Hall India Learning Private Limited.
1. 7.Arnikar, H.J., (1987), Second Edition, **Essentials of Nuclear Chemistry,** Wiley Blackwell Publishers
7. Arnikar, H.J.; Rajurkar, N. S.,(2016) **Nuclear Chemistry through Problems,** New Age International Pvt. Ltd.
8. De, A.K.(2012), **Environmental Chemistry,** New Age International Pvt., Ltd.
9. Khopkar, S.M.(2010), **Environmental Pollution Analysis**, New Age International Publisher.
10. Das, A. K. (2010), ***Fundamentals of Inorganic Chemistry***, Volume 1, Second Edition, CBS Publishers & Distributors Pvt Ltd.
11. Das, A. K. (2012), ***Environment Chemistry with Green chemistry***, Books and Allied (P) Ltd.


**Practical:**


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


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

## DISCIPLINE SPECIFIC ELECTIVE COURSE – 5 (DSE-5): Reactions, Reagents and Chemical Process

### 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 | | |
| **Reactions, Reagents and Chemical Process (DSE-5)** | 04 | 03 | -- | 01 | Class $12^{th}$ with Physics, Chemistry | Basic knowledge of organic reactions |

### Learning objectives

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

- To study the important organic name and rearrangement reactions that are crucial for the synthesis of valuable organic compounds.
- To give the knowledge belonging to the role of reagents in organic reactions for the synthesis of chemo-, diastereo- and enantio-selective products.
- To impart the knowledge of process chemistry that is a key part of the large-scale synthesis of chemical products essential for day-to-day life

### Learning outcomes

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

- Explain the reaction mechanism of various name and rearrangement reactions
- Discuss the role of the reagents in organic synthesis and apply these reagents for the bulk chemical synthesis
- Debate and use oxidizing and reducing reagents for selective synthesis organic products
- Apply the learnt techniques to chemical processes
- Acquire skills for human resource building especially in the chemical industry.

### SYLLABUS OF DSE-5

**UNIT – 1: Name Reactions** **(15 Hours)**

Application, scope and mechanism of following reactions: Prevost Reaction, Chugaev Reaction, Maukaiyama Aldol Reaction, Mozingo Reaction, Ramberg Backlund Reaction, Shapiro Reaction, Barbier Reaction, Clark- Eschweiler Reaction, Darzen’s Reaction, Julia-Olifination Reaction, Tiffeneaus Damjanov Reaction, Darkin West Reaction, Bischler-Napieralaski Reaction, Birch reduction of aromatic compounds, Appel Reaction, Mitsunobu

Reaction, Corey Kim Oxidation, Azide-alkyne 1,3-dipolar cycloaddition reaction, Olefin metathesis: Grubbs reaction, Heck Reaction, Suzuki coupling and Wittig reaction.

**UNIT – 2: Reducing Reagents** **(9 Hours)**

Reactions, mechanism and applications of following reducing agents: Sodium borohydride, Lithium aluminium hydride, $NaBH_3CN$, DIBALH, lithium-tri-*tert*-butoxyaluminum hydride, Red-Al $Na[AlH_2(OCH_2OCH_2OCH_3)_2]$, Zinc borohydride, L and K selectrides, $LiBHEt_3$ and $KBHEt_3$, Luche Reagent $NaBH_4$-$CeCl_3$, $K[BH(OAc)_3]$, *bis*-Boric Acid (BBA), Catecholborane, DEMS (Diethoxymethylsilane), 3-Mercapto propionic acid, Polymethylhydrosiloxane (PMHS), Schwartz's Reagent (Zirconocene chloride hydride).

**UNIT – 3: Oxidizing Reagents** **(9 Hours**

Reactions, mechanism and applications of following oxidizing agents: Jones Reagent ($CrO_3$, $H_2SO_4$, $H_2O$), Swern Reagent (DMSO, oxalyl chloride), Dess Martin, TEMPO, TPAP (Tetrapropyl ammonium perruthenate), Fetizon's Reagent, Fenton's Reagent [$H_2O_2$ + Fe(II) ion], Sodium perborate $NaH_2BO_4$, Sodium Bismuthate $NaBiO_3$, ABNO (9-Azabicyclo[3.3.1]nonane N-oxyl), DEAP (Diethyl allyl phosphate, 

), AZADO (2-Azaadamantane N-oxyl], Wacker oxidation.

**UNIT – 4: Process Chemistry** **(12 Hours)**

1. Process chemistry a) Introduction, stages of scale up process: Bench, pilot, and large-scale process with at least two examples of scale up process of API. b) In-process control and validation of large-scale process.
2. Unit Processes: The following unit processes should be studied with mechanism and one example of each process Nitration: Nitrating agents, process equipment for technical nitration. Halogenation: Types of halogenations, catalytic halogenations. Reduction: Catalytic hydrogenation, hydrogen transfer reactions, metal hydrides. Oxidation: Types of oxidative reactions, and non-metallic oxidizing agents such as H, sodium hypochlorite, oxygen gas, ozonolysis.

## Practical component **Credits:**

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

1. Oxidation of alcohols to acid using Jones reagent.
2. Reduction of acetophenone and its derivatives to 1-phenyl ethanol derivatives by $NaBH_4$.
3. Reduction of 4-tert-butyl-cyclohexanone to cis and trans 4-tert-butyl-cyclohexanol.
4. Synthesis of 2,5-dimethyl-2,5-hexanediol from tert-butanol using Fenton's reagents.
5. Wittig reaction of benzyltriphenylphosphonium chloride and 4-bromobenzaldehyde using potassium phosphate (tribasic).
6. Substitution ($S_N2$) reaction of 1-iodobutane and 2-naphthol.
7. Aldol condensation reaction: solventless synthesis of chalcones.
8. Borohydride reduction of a ketone: hydrobenzoin from benzil.
9. Visit to chemical industry of the demonstration of pilot scale.

**Essential/recommended readings**

**Theory:**

2. Clayden, J. Greeves, N., Warren, S. **Organic Chemistry**, South Asian Edition, Oxford University Press, USA
3. Gadamasetti K., **Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever- Changing Climate-An Overview**, Vol-2, CRC Press, London.
4. Murphy R.M., **Introduction to Chemical Processes: Principles, Analysis, Synthesis**, McGraw-Hill Education, New York.
5. Harrington P. J., **Pharmaceutical Process Chemistry for Synthesis: Rethinking the Routes to Scale up**, John Wiley and Sons, Inc, New Jersey.
6. Parashar, R.K.; Ahluwalia, V.K. (2018), **Organic Reaction Mechanism,** 4th Edition, Narosa Publishing House.

**Practical:**

1. Mann F.G, Saunders, B.C., **Practical Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.
2. Vogel A.I., **Elementary Practical Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.

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

## DISCIPLINE SPECIFIC ELECTIVE COURSE - 6 (DSE- 6): Polymers, Colloids, Surfaces and Interfaces

### 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 | | |
| **Polymers, Colloids, Surfaces and Interfaces (DSE- 6)** | **04** | **03** | **--** | **01** | Class 12th with Physics, Chemistry | **--** |

### Learning Objectives

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

- To give students a comprehensive coverage of important physical aspects of polymers chemistry, colloids, emulsions, surfaces and interfaces.
- to study the applications of these aspects.

### Learning outcomes

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

- Explain the types of polymers, kinetics of polymerization and polymer properties.
- Understand and apply the concepts of properties of polymer solutions and their thermodynamics.
- Comprehend the basic concepts of surface chemistry specifically in relation to colloids.
- Have a thorough understanding of applications of colloids in various areas.

### SYLLABUS OF DSE-6

**UNIT 1: Introduction to polymers (Hours: 6)**

Recapitulation of basic concepts of polymers. Types of polymerizations and their mechanism and kinetics: Free radical, ionic, step-growth, coordination, copolymerization. Polymerization techniques: Bulk, solution, suspension, and emulsion.

**UNIT 2: Polymer solution (Hours: 9)**

Polymer solution – solubility parameter, properties of dilute solutions and their criteria, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change. Flory Huggins theory.

**UNIT 3: Introduction to Colloid Chemistry** **(Hours: 9)**

Recapitulation of basic concepts of Adsorption, 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), preparation and properties of colloids - Tyndall effect, Brownian movement, electrophoresis, dialysis, coagulation and flocculation; Charge on Colloidal particles and Electrical double layer concept, Suspensions and their characteristics, Emulsions and their characteristics.

**UNIT 4: Surface chemistry in relation to colloids** **(Hours: 12)**

Surface film on liquid surface, surface potential, monomolecular films, Langmuir Blodgett layers. Emulsions, foams and aerosols; electrical aspects of surface chemistry; Surface of solids, solid-liquid interface, stability of dispersions, stabilization of suspensions

**UNIT 5: Application of colloids** **(Hours: 9)**

Characterization of colloidal particles, Role of colloid chemistry in Nanotechnology (wet colloid chemical approach, "bottom up" fabrication of nanoparticles and nanostructured materials), applications of colloid chemistry in petroleum recovery, coating and painting, food, pharmaceuticals and cosmetic industry, medicinal chemistry (use in drug formulations), Sewage disposal, Purification of water, cleansing action of soap, Formation of Delta, Smoke precipitation, Photography, Artificial rain

**Practical component**

## Practicals: Credits: 01

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

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA)/MethylAcrylate (MA).
2. Preparation of nylon 6,6
3. Determination of molecular weight of polyvinyl propylidene in water by viscometry.
4. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of head-to-head monomer linkages in the polymer.
5. Determination of molecular weight by end group analysis of polymethacrylic acid.
6. Estimation of the amount of HCHO in the given solution by sodium sulphite method.
7. Preparation of Colloidal Sols of following
   A. Arsenic sulphide,

B. Antimony sulphide

C. Ferric chloride

D. Aluminium hydroxide

8. To find out the precipitation values of arsenious sulphide sol by using monovalent, bivalent and trivalent cations.
9. To determine the nature of charge on particle in given colloidal solution and their electrophoretic velocity and zeta potential.
10. To prepare lyophilic sol of starch.

**Essential/recommended readings**

**Theory:**


1. Carraher,C. E. Jr. (2013), **Seymour's Polymer Chemistry**, Marcel Dekker, Inc.
2. Odian, G. (2004), **Principles of Polymerization**, John Wiley.
3. Billmeyer, F.W. (1984), **Text Book of Polymer Science**, John Wiley
4. Myers D.,Surface, interfaces and colloids Principles and Applications, 2nd Edition, Wiley-VCH
5. V.R. Gowarikar (2010), **Polymer Science**, New Age International Publishers Ltd.


**Practical:**


1. Sperling, L.H. (2005), **Introduction to Physical Polymer Science**, John Wiley & Sons


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

## DISCIPLINE SPECIFIC ELECTIVE COURSE -7 (DSE-7): Novel Inorganic Solids

### 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 | | |
| **Novel Inorganic Solids (DSE-7)** | 04 | 03 | -- | 01 | Class 12th with Physics, Chemistry | -- |

### Learning Objectives

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

- To familiarize the students with the characterization techniques of inorganic solids
- To familiarize the students with use and manifold applications of composites, carbon or high-tech ceramics

### Learning Outcomes:

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

- Explain the mechanism of solid-state synthesis.
- Explain about the different characterization techniques and their principle.
- Explain the importance of composites and their applications.
- Discuss and explain the usage of solid materials in various instruments, batteries, etc. which would help them to appreciate the real-life importance of these materials

### SYLLABUS OF DSE- 7

**Unit 1: Synthesis of inorganic solids (Hours: 5)**

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

**Unit 2: Characterization techniques of inorganic solids (Hours: 10)**

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

**Unit 3: Pigments** **(Hours: 10)**

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

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

**Unit 4: Composite materials** **(Hours: 10)**

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

**Unit 5: Speciality polymers** **(Hours: 10)**

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

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

**Practicals** **Credits: 01**

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

1. Preparation of polyaniline and its characterization using UV-visible spectrophotometer.
2. Intercalation of hydrogen in tungsten trioxide and its conductivity measurement using conductometer.
3. Synthesis of the following inorganic pigments:

   (i) $PbCrO_4$ / chrome yellow

   (ii) Barium white

   (iii) Prussian Blue

   (iv) Malachite

. 4.- Preparation of zeolite A and removal of Mg and Ca ions from water samples quantitatively using zeolite.

5. Determination of exchange capacity of cation exchange resins and anion exchange resins.

6. Determination of a mixture of cobalt and nickel (UV-visible spectroscopy).
7. Preparation of a disc of a ceramic compound using ball milling, pressing and sintering, and study its XRD.

**Essential/recommended readings**

**Theory:**


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


**Practicals:**


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


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

## DISCIPLINE SPECIFIC ELECTIVE COURSE – 8 (DSE-8): Applied 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 | | |
| Applied Organic Chemistry (DSE-8) | 04 | 03 | -- | 01 | Class 12$^{th}$ with Physics, Chemistry | -- |

### Learning Objectives

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

- To make students aware of the importance of organic compounds in daily life.
- To familiarize students with the chemistry and uses of dyes, polymers, terpenoids, alkaloids, steroids and pharmaceutical compounds and their direct or indirect effect on human life and health

### Learning outcomes

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

- Discuss and demonstrate the chemistry and uses of commercially important and naturally occurring compounds like dyes, polymers, terpenoids, alkaloids, steroids and pharmaceuticals.
- Appreciate the chemistry of biodegradable and conducting polymers and their importance to human life and society.
- Comprehend the chemistry of dyeing and dyes. Explain why some dyes are better than others. Describe the applications of various types of dyes including those in foods and textiles.
- Comprehend the synthetic routes and mode of action of some selected pharmaceutical compounds
- Use the knowledge gained to solve real world problems

## SYLLABUS OF DSE-8

**Unit 1: Dyes (Hours: 7)**

Nomenclature of commercial dyes with at least one example. Suffixes - G, O, R, B, 6B, L, S; colour index and colour index number. Classification of dyes based on structure and application; Chemistry of dyeing.

Synthesis and applications of the following types of dyes: Azo dyes - Methyl orange, Congo red; Triphenyl methane dyes-Malachite green, Rosaniline and Crystal violet; Phthalein Dyes - Phenolphthalein; Natural dyes - Structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes (natural and synthetic) with examples and effect of synthetic food colours on health.

**Unit 2: 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 (Tg) 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 3: Natural Product Chemistry- An Introduction to Terpenoids, Alkaloids and Steroids (Hours: 12)**

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.

Steroids: Introduction, occurrence, structure, Diel's hydrocarbon, nomenclature of steroid hydrocarbons, structure and biological functions of the following steroids- Cholesterol, Sex Hormones (Estrogen, androgen and progesterone), Adrenocortical hormones (Cortisone and cortisol) and Ergosterol (antirachitic effect).

**Unit 4: Pharmaceutical Compounds** **(Hours:14)**

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

Antipyretics -Paracetamol; Analgesics- Ibuprofen; Antimalarials - Chloroquine; Antitubercular drugs - Isoniazid.

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

**Practical component**

**Practical:** **Credits: 01**

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

**(At least five experiments to be performed)**

1. Synthesis of urea formaldehyde resin and test the solubility.
2. Preparation of Starch-PVA Film.
3. Preparation of Methyl orange.
4. Separation of a mixture of dyes by Thin Layer Chromatography (TLC).
5. Isolation and estimation of the content of aspirin in a commercial tablet.
6. Synthesis of 4-methyl-7-hydroxycoumarin by condensation of resorcinol with ethyl acetoacetate.
7. Synthesis of 3,5-dimethyl pyrazole by condensation of acetylacetone and hydrazine.
8. Synthesis of benzimidazole.
9. Synthesis of 2,3-diphenylquinoxaline.
10. Synthesis of paracetamol

**Essential/recommended readings**

**Theory:**

1. Finar, I.L. Fifth Edition **Organic Chemistry**, Volume 2, Pearson Education, 2008.
2. Saunders, K. J., (1988), **Organic Polymer Chemistry,** Second Edition Chapman & Hall, London.
3. Campbell, Ian M., (2000), **Introduction to Synthetic Polymers**, Second 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), Fourth Edition, Oxford University Press.
6. Beale J.M. Block J., (2010) **Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry,** Twelfth Edition, Lippincott Williams and Wilkins.
7. Alagarsamy, V. (2010), **Textbook of Medicinal Chemistry**, Volume II, Second Edition, Reed Elsevier India Private Limited.

**Practical:**


1. Sciam, A.J. **TLC of mixture of dyes**; *J. Chem. Educ*., **1985**, 62(4), 361. https://pubs.acs.org/doi/10.1021/ed062p361.
2. McKone, H.T.; Nelson, G.J**. Separation, and identification of some FD &C dyes by TLC. An undergraduate laboratory experiment**, *J. Chem. Educ*., **1976**, *53*(11), 722. DOI: 10.1021/ed053p722.


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

## DISCIPLINE SPECIFIC ELECTIVE COURSE- 9 (DSE-9): Applications of Computers 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 | | |
| **Applications of Computers in Chemistry (DSE 9)** | **04** | **03** | **-** | **01** | Class 12$^{th}$ with Physics, Chemistry | |

### Learning Objectives

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

- To familiarize the students with the fundamental building blocks and syntax of coding in Python with
- To apply python programming to solve simple Chemistry problems by thinking algorithmically and coding structurally

### Learning outcomes

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

- Understand the importance of python programming in chemistry and its applications in the field of AI and ML
- Perform simple computations in python after learning the basic syntax, loop structure, string data manipulation etc.
- Solve chemistry problems such as finding pKa of a weak acid, solving Schrodinger's equation etc.
- Plot experimental data and perform regression analysis

### SYLLABUS OF DSE-9

**UNIT–1: Basic Computer system** **(Hours: 3)**

Hardware and Software; Input devices, Storage devices, Output devices, Central Processing Unit (Control Unit and Arithmetic Logic Unit); Number system (Binary, Octal and

Hexadecimal Operating System); Computer Codes (BCD and ASCII); Numeric/String constants and variables. Operating Systems (DOS, WINDOWS, and Linux); Software languages: Low level and High-Level languages (Machine language, Assembly language; QBASIC, C, C++, FORTRAN 90&95); Compiled versus interpreted languages. Debugging Software Products (Office, chemsketch, scilab, matlab, and hyperchem), internet application

**UNIT-2: Introduction to Python** **(Hours: 3)**

Why Python? Python coding environment setup, Python as an interpreted language, Brief history of Python, Uses of Python (including artificial intelligence and machine learning), Applications of Python in Chemistry

**UNIT-3: Coding in Python** **(Hours: 18)**

(i) Basic syntax including constants and variables, Operators, Data Types, Declaring and using Numeric data types: int, float, string etc. (ii) Program Flow Control Conditional blocks: if, else and else if, simple FOR loops, FOR loop using ranges, string, list and dictionaries. Use of while loops, Loop manipulation using pass, continue, break and else. (iii) Complex data types: String, List, Arrays, Tuples and Dictionary, String operations and manipulation methods, List operations including slicing, in-built Python Functions. (iv) Python packages - usage of numpy and scipy for mathematical computations.

**UNIT-4: Plotting graphs** **(Hours: 9)**

Matplotlib for Plotting - Simple plots, formatting of plots, multiple plots, histograms, bar graphs, distributions, curve fitting – linear regression.

**UNIT-5: Numerical Methods in Chemistry** **(Hours: 12)**

Solution of quadratic equation, polynomial equations (formula, iteration, Newton – Raphson methods and binary bisection) with examples of polynomial equations used in chemistry; Numerical differentiation – finite difference method (backward, central and forward), Numerical integration - Trapezoidal and Simpson's rule to calculate area under the curves for chemistry problems, e.g., entropy calculations, Simultaneous equations, Statistical analysis-mean, variance, standard deviation, error, Curve fitting – linear regression, Solving Schrödinger's equation using Python packages.

**Practical component**

**Practicals: Python Programming for Chemists** **Credits: 01**

4. **Writing simple programs using scipy and numpy**
    a. syntax, data types
    b. loop structure, conditional loops

c. To learn string data manipulation
d. Array and lists
e. Sorting, matrix manipulations

5. **Plotting graphs using matplotlib**
    a. Planck's distribution law
    b. Maxwell-Boltzmann distribution curves as a function of temperature and mass
    c. Radial distribution curves for hydrogenic orbitals
    d. Gas law Isotherms – Ideal and Real
    e. Data from phase equilibria studies
    f. Wavefunctions and Probabilities as multiplots
    g. Kinetics data with linear fitting

6. **Numerical Methods in Chemistry**
    a. Solving equations involved in chemical equilibria such as pH of a weak acid at a given concentration, cubic equation obtained from solving van der Waals equation of real gases using Iteration, Newton-Raphson, and Binary Bisection Method
    b. Numerical Differentiation – finding equivalence point given pH metric and potentiometric titrations data by finding the first and the second derivative using the finite difference method
    c. Numerical Integration – Trapezoidal and Simpson's 1/3 rule to calculate enthalpy and entropy of an ideal gas
    d. Statistical Analysis – Calculating Mean, Variance, Standard Deviation
    e. Solving Schrodinger's Equation

**Essential/recommended readings**

**Theory:**

7. Dr. M. Kanagasabapathy(2023), **Python for Chemistry: An introduction to Python algorithms, Simulations, and Programing for Chemistry** (English Edition), BPB Publications
8. Robert Johansson (2021), **Numerical Python: Scientific Computing and Data Science Applications with Numpy, SciPy and Matplotlib**, 2nd Edition, Apress

**Practical**

1. Urban M., Murach J., **Murach's Python programming,** 2nd Indian reprint 2018, Shroff publishers and distributors
2. Gaddis T., **Starting out with python plus My programming Lab** with Pearson e-text-Access card package, 3rd ed.

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

## DISCIPLINE SPECIFIC ELECTIVE COURSE - 10(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 | | |
| Analytical Methods in Chemistry (DSE-10) | 04 | 03 | -- | 01 | Class 12th with Physics, Chemistry | - |

### Learning Objectives

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

- To familiarize the students with concept of sampling, Accuracy, Precision, Statistical test data-F, Q and t test.
- To familiarize the students with the laws of spectroscopy and selection rules governing the possible transitions in the different regions of the electromagnetic spectra.
- To familiarize the students with important separation methods like solvent extraction and chromatography

### Learning Outcomes:

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

- Perform experiment with accuracy and precision.
- Develop methods of analysis for different samples independently.
- Test contaminated water samples.
- Use basic principle of instrument like Flame Photometer, UV-Visible spectrophotometer learnt for practical applications.
- Apply knowledge of geometrical isomers and keto-enol tautomers to analysis.
- Determine composition of soil.
- Estimate macronutrients using Flame photometry.

## SYLLABUS OF DSE-10

**Unit 1: Qualitative and Quantitative Aspects of Analysis: (Hours: 5)**

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

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

**Unit 2: Optical Methods of Analysis (Hours: 25)**

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

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

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

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

**Unit 3: Thermal methods of analysis (Hours: 5)**

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

**Unit 4: Separation techniques (Hours:10)**

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

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

Chromatography: Classification, principle and efficiency of the technique, Mechanism of separation: adsorption, partition & ion-exchange

**Practicals Credits 01**

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

1. Separation of constituents of leaf pigments by Thin Layer Chromatography

2. Solvent Extractions

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

3. Analysis of soil:

   (i) Total soluble salt
   (ii) Estimation of exchangeable calcium and magnesium
   (iii) Estimation of carbonate and bicarbonate
   (iv) Qualitative detection of nitrate and phosphate

4. Separation of amino acids from organic acids by ion exchange chromatography.
5. Spectrophotometry

   (i) Verification of Lambert-Beer's law and determination of concentration of a coloured species ($CuSO_4$ / $KMnO_4$ /$CoCl_2$ / $CoSO_4$)
   (ii) Spectrophotometric analysis of caffeine and benzoic acid in a soft drink
   (iii) Determination of concentration of coloured species via following methods;
   (a) Graphical method, (b) Epsilon method, (c) Ratio method, (iv) Standard addition method

6. Flamephotomerty
   (i) Estimation of potassium, calcium and magnesium using flame photometry

**Essential/recommended readings**

**Theory:**

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

**Practicals:**

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

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

# DISCIPLINE SPECIFIC ELECTIVE COURSE - 11 (DSE-11): Basic Principles of Food 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 Principles of Food Chemistry (DSE-11) | 04 | 03 | -- | 01 | Class 12$^{th}$ with Physics, Chemistry | -- |

## Learning Objectives

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

- To make students understand the sources, importance, stability and transformations of food components during handling and processing.
- To make students aware about nature and importance of additives in food chemistry.

## Learning outcomes

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

- Develop a strong understanding of basic fundamentals of food chemistry
- Discuss and demonstrate how alterations /transformations during processing and handling affect the quality and stability of food
- Develop an elementary idea on the nature and importance of additives in food chemistry.
- Apply the knowledge gained to real world problems

## SYLLABUS OF DSE-11

**Unit 1: Introduction** **(Hours:3)**

What is food chemistry; An overview of the following: alterations during handling or processing (texture, flavour, colour), chemical and biochemical reactions leading to alteration in food quality (browning, oxidation, hydrolysis, protein denaturation), cause and effect relationship pertaining to food handling; factors governing stability of food (chemical and environmental factors) and role of food chemists.

**Unit 2: Water** **(Hours:3)**

Definition of water in food, structure of water and ice, types of water, sorption phenomenon, water activity and packaging, water activity and shelf-life.

**Unit 3: Carbohydrates (Hours:6)**

Introduction, sources, functions, deficiencies, structure and importance of polysaccharides in food chemistry (Agar and Agarose, Pectin, Hemicellulose, Cyclodextrins, Gums, Alginate, Starches, modified starches), Non-enzymatic browning and its prevention, caramelisation, formation of acrylamide in food, role of carbohydrates as sweeteners and comparison with artificial sweeteners.

**Unit 4: Proteins (Hours:6)**

Introduction, sources, classification, functions, deficiencies, physico-chemical & functional properties of proteins, nature of food proteins (plant and animal proteins).

**Unit 5: Lipids (Hours:6)**

Introduction, sources, classification and physical properties, functions, deficiencies, effect of frying on fat, reaction of lipids: hydrogenation, interesterification, hydrolysis, auto-oxidation and its prevention; flavour reversion, fat replacers: fat mimetics and fat substitutes.

**Unit 6: Vitamins and Minerals (Hours:6)**

Vitamins: Introduction, sources, classification: water soluble and water insoluble vitamins, essential vitamins, physiological function, deficiencies, causes of variation and loss in foods, vitamin like compounds, effect of food processing.

Minerals: Introduction, sources, classification: major minerals and trace elements, physiological function, deficiencies, factors affecting mineral content of food, fortification and enrichment of foods with minerals, effect of food processing.

**Unit 7: Food Additives (Hours:15)**

Additives: Introduction, importance, classification, antioxidants, emulsifiers, stabilizers, gelling agents, gums, thickeners, sweeteners, acidulants, preservatives, humectants, food toxins

Colouring Agents and Pigments: Introduction, natural food colourants: anthocyanins, carotenoids, chlorophyll, caramel, betalains; examples of pigments in common food; Nature-identical colourants: $\beta$-Carotene, canthaxanthin and riboflavin; artificial colouring agents; artificial/synthetic colourants: Azo dyes (e.g. amaranth dye, tatrazine, citrous red, Allura red); quinoline (e.g. quinoline yellow); phthalein (e.g. erythrosine); triarylmethanes and indigoid (e.g. indigo carmine), FD&C Dyes and lakes; properties of certified dyes, colours exempt from certification.

Food Flavor: Sensation of taste and odour, chemical dimension of basic types of taste (Salty, Sweet, Bitter, Sour, Umami taste), other sensations like astringency, coolness, pungency/pungency); non-nutritive sweeteners (aspartame, saccharin, sucralose, cyclamate) and nutritive sweeteners, molecular mechanism of flavour perception, biogenesis of fruits and vegetable flavors, taste inhibition, modification and enhancement, common vegetable and spice flavors.

**Practical component**

**Practical:** **Credits: 01**

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

**(At least four experiments to be performed)**

1. Determination of moisture in food products by hot air oven-drying method.
2. Paper chromatography of synthetic food dyes.
3. Quantitative determination of food dyes in powdered drink mixes by spectrophotometric method.
4. Colorimetric determination of Iron in vitamin / dietary tablets.
5. Determination of rancidity of edible oils by Kriess Test.
6. Estimation of Vitamin C in a given solution/ lemon Juice/chillies by 2, 6-dichlorophenol by Indophenol Method.
7. Isolation of casein from milk.
8. Qualitative estimation of cholesterol by Liebermann-Burchard method.
9. Detecting the presence of Vanaspati and rancidity in the given Ghee sample through qualitative tests.

**Essential/recommended readings**

**Theory:**


1. DeMan, J.M., Finley, J.W., Hurst, W.J., Lee, C.Y. (2018), **Principles of Food Chemistry**, Fourth Edition, Springer.
2. Msagati, T.A.M. (2013), **Chemistry of Food Additives and Preservatives**, Wiley-Blackwell.
3. Fennema, O.R. (2017), **Food Chemistry**, Fifth Edition, CRC Press.
4. Attokaran, M. (2017), **Natural Food Flavors and Colorants**, Second Edition, Wiley-Blackwell.
5. Potter, N.N., Hotchkiss, J.H, (1995) **Food Science,** Fifth Edition, Chapman & Hall.
6. Brannen, D., Davidsin, P.M., Salminen, T. Thorngate III, J.H. (2002), **Food Additives**, Second Edition, CRC Press.
7. Coultate, T. (2016), **Food: The Chemistry of its Components**, Sixth Edition, Royal Society of Chemistry.
8. Belitz, H. D.; Grosch, W. (2009), **Food Chemistry**, Springer.
9. Course: Food Chemistry (iasri.res.in)


**Practical:**


1. Ranganna, S. (2017). **Handbook of analysis and quality control for fruits and vegetable products**, Second Edition, McGraw Hill Education
2. Sawhney, S.K., Singh, R. (2001), **Introductory Practical Biochemistry**, Narosa Publishing House

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

## DISCIPLINE SPECIFIC ELECTIVE COURSE -12 (DSE-12): Computational Methods & Molecular Modelling

### 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 | | |
| **Computational Methods & Molecular Modelling (DSE-12)** | **04** | **03** | **--** | **01** | Class 12th with Physics, Chemistry and Mathematics | **--** |

### Learning Objectives

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

- To make students learn the theoretical background of computational techniques in molecular modelling.
- To give the different flavours of computational chemistry by the end of this course.
- To provide hands-on experience in molecular modelling on various software

### Learning outcomes

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

- Explain the theoretical background of computational techniques and selective application to various molecular systems.
- Compare computational and experimental results and explain deviations.
- Perform Optimization of geometry parameters of a molecule (such as shape, bond length and bond angle) through the use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.
- Perform analysis of molecular properties using various software.

## SYLLABUS OF DSE-12

**UNIT-1 : Introduction** **(Hours: 6)**

Introduction to computational chemistry: Overview of Classical and Quantum Mechanical Methods (Ab initio, DFT, Semi-empirical, Molecular Mechanics, Molecular Dynamics, and Monte Carlo)

**UNIT – 2: Potential Energy Surfaces** **(Hours: 6)**

Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global minima, Geometry optimization and energy minimization, the concept of transition state with examples, Hessian matrix

**UNIT – 3 : Molecular Mechanics & Molecular Dynamics** **(Hours: 9)**

***Molecular Mechanics***

Force Fields (A brief explanation of all the terms of a basic force field), the basic idea of MM1, MM2, MM3, MM4, MM+, AMBER, BIO+, OPLS.

***Molecular Dynamics***

The concept of the periodic box, ensembles (microcanonical, canonical, isothermal – isobaric), steps in a typical MD simulation.

**UNIT-4: Huckel Molecular Orbital Theory** **(Hours: 6)**

Huckel MO with examples: ethene and propenyl systems, Properties calculated – energy, charges, bond order, electronic energies, resonance energies.

**UNIT- 5: Computational Methods** **(Hours: 18)**

***Ab-initio methods***
Antisymmetry principle, Slater determinants, SCF method, Hartree-Fock method.
Basis sets, Basis functions, STOs and GTOs, diffuse and polarization functions. Minimal basis sets, Basis set superposition error (BSSE) - Effective core potentials (ECP)
Advantages of ab initio calculations.

***Density Functional Theory***
A brief description of Density Functional Theory (DFT). Calculation of Electronic Properties in ground and Excited states

***Semi-empirical methods***
Basic idea about Zero differential overlap (ZDO) approximation

***Some important concepts***

Concepts of atomic charges, electrostatic potential maps, computation of thermodynamic properties and spectroscopic observables

**Practical component**

**Practical:** **Credits: 01**

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

1) Write the Z-Matrix of a given set of molecules.

2) Carry out geometry optimisation on $H_2O$, $H_2S$, $H_2Se$ molecules compare the optimized bond angles and dipole moments from the results obtained. Obtain the ESP-mapped density surfaces and interpret the results obtained with reference to bonding in these molecules.

   Suggestive: A comparative analysis of results of the above exercise may be carried out using different quantum mechanical methods.

3) Calculate the energy of the following chemical species and arrange them in order of increasing stability.

   1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3- dimethyl-2-butene in order of increasing stability.

4) Carry out geometry optimisation on the following chemical species and compare the shapes and dipole moments of the molecules.

   1-pentanol, 2-pentanol, 3-pentanol, 2-methylbutan-1-ol, 3-methylbutan-1-ol, 2-methylbutan-2-ol, 2-methylbutan-3-ol and 2,2-dimethylpropanol.

   Correlate the computationally obtained values of the dipole moments with the experimental values of the boiling points: (118 ºC, 100 ºC, 108 ºC, 82 ºC, of 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2- propanol respectively).

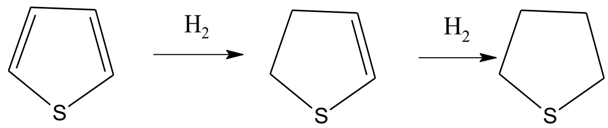
5) Based on the implicit electronic structure calculations, determine the heat of hydrogenation of Propylene.

6) Based on the calculations of enthanlies of the participating chemical species on optimized geometry of the molecules, calculate the reaction enthalpy at 298 K for the following, industrially important reactions:

   $$CH_4 + H_2O \rightarrow CO + 3H_2 \text{ (steam reforming of methane)}$$

   ≡≡ (Haber-Bosch process)

7) Carry out geometry optimisation and determine the energy of the participating chemical species in the following reactions Using these results calculate the resonance energy of thiophene.




8) Carry out geometry optimisation & Energy calculations on the following species and obtain Frontier Molecular Orbitals. Visualize the Molecular Orbitals of these species and interpret the results for bonding in these molecules.
Benzene, Naphthalene, and Anthracene.

9) Compare the gas phase basicities of the methylamines by comparing the enthalpies of the following reactions:

$$BH^{+} + NH_3 \rightarrow B + NH_4^{+}$$

Where B = $CH_3NH_2$, $(CH_3)_2NH$, $(CH_3)_3N$

10) On the basis of results of geometry optimization and energy calculations, determine the enthalpy of isomerization of cis and trans 2-butene.

11) Perform a conformational analysis of butane. Plot the graph between the angle of rotation and the energy of the conformers using spreadsheet software.

12) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.

13) Calculate the electronic UV/Visible absorption spectrum of Benzene.

14) Calculate the electronic absorption spectra of formaldehyde.

15) Plot the electrostatic potential mapped on electron density for benzene and use it to predict the type of stacking in the crystal structure of benzene dimer.

16) On a given set of molecules methylamine ($CH_3NH_2$) carry out geometry optimization, single point energy and NBO calculations and interpret the output results treated at the ab initio RHF/3-21G level.

17) Study the mechanism of $SN_2$ reaction between $Cl^-$ and $CH_3Br$ involving a Walden inversion computationally.

18) Perform a geometry optimization followed by a frequency assessment (opt+freq keyword) using the B3LYP method and 6-31-G(d) basis set on a given set of small molecules i.e. $BH_3$, $CH_4$.
**Suggestive:** A greater number of molecules may be studied as per instructions received from the concerned teacher.

19) Based on the fundamentals of conceptual DFT calculate the ionization potential (IP), electron affinity (EA), electronegativity and electron chemical potential of a given set of molecules.

20) Perform molecular docking of Sulfonamide-type D-Glucose inhibitor into MurrD active site using Argus Lab.

21) Perform molecular dynamics (MD) simulation of a given alkali metal ion in aqueous function (RDF)

**Essential/recommended readings**

**Theory:**


1. Lewars, E. (2003), **Computational Chemistry**, Kluwer academic Publisher.
2. Cramer, C.J. (2004), **Essentials of Computational Chemistry**, John Wiley & Sons.
3. Hinchcliffe, A. (1996), **Modelling Molecular Structures**, John Wiley & Sons.
4. Leach, A.R. (2001), **Molecular Modelling**, Prentice-Hall.
5. House, J.E. (2004), **Fundamentals of Quantum Chemistry**, 2nd Edition, Elsevier.
6. McQuarrie, D.A. (2016), **Quantum Chemistry**, Viva Books.
7. Levine, I. N.; **Physical Chemistry**, 5th Edition, McGraw –Hill.


**Practical:**


1. https://www.afs.enea.it/software/orca/orca_manual_4_2_1.pdf
2. https://dasher.wustl.edu/chem430/software/avogadro/learning-avogadro.pdf
3. http://www.arguslab.com/arguslab.com/ArgusLab.html
4. https://barrett-group.mcgill.ca/tutorials/Gaussian%20tutorial.pdf
5. https://gaussian.com/techsupport/
6. https://gaussian.com/man/
7. https://gaussian.com/wp-content/uploads/dl/gv6.pdf
8. https://dasher.wustl.edu/chem478/software/spartan-manual.pdf
9. http://www.mdtutorials.com/gmx/
10. https://vina.scripps.edu/manual/


**Important Instruction Note on working approach:**

- A student is required to perform/investigate a minimum of 10 exercises from the given set of exercises.
- The students may use open source softwares; ArgusLab, Avogadro and ORCA. In case a licenced version softwares is available, if procured by the college, other licenced softwares may also be used.

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

## 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 | | |
| **Research Methodology for Chemists (DSE-13)** | 04 | 03 | -- | 01 | Class 12th 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, Chemsketch 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 dublications

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** **(Hours: 6)**

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 Chemsketch 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


**Note:**

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

- **The students are required to opt one paper each from DSEs 1-3 in Semester 3, DSEs 4-6 in Semester 4, DSEs 7-9 in Semester 5 and DSEs 10-13 in Semester 6.**

- **Research Methodology (DSE 13) shall be offered as one of the DSE courses in semester VI or VII. If a student wishes to pursue four years Honours Degree with Research, he/she shall compulsorily opt for a Research Methodology course in either Semester VI or VII.**

BSC. (PHYSICAL SCIENCES)- CHEMISTRY COMPONENT

**SEMESTER - IV**

## DISCIPLINE SPECIFIC CORE COURSE CHEM-DSC -10: Chemistry- IV: Chemistry of Carboxylic Acids & their Derivatives, Amines and Heterocycles

### 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 | | |
| **Chemistry of Carboxylic Acids & their Derivatives, Amines and Heterocycles DSC-10: Chemistry-IV** | **04** | **02** | **-** | **02** | **Class 12th with Physics, Chemistry, Mathematics** | |

### Learning Objectives

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

- To make students learn about the chemistry of carboxylic acids and their derivatives (aliphatic and aromatic)
- To give basic understanding of amines (aliphatic & aromatic), diazonium salts
- To provide basic understanding of heterocyclic systems.

### Learning outcomes

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

- Understand reactions of carboxylic acids, esters, amides, amines and diazonium salts
- Understand the concept of protection and deprotection.
- Use the synthetic chemistry learnt in this course to do functional group transformations.
- Gain theoretical understanding of chemistry of heterocyclic compounds.

### Syllabus

**Unit 1: Carboxylic Acids and their Derivatives (aliphatic and aromatic) ( 1 3 Lectures)**

Preparation: Oxidation reactions of alcohols, aldehydes and ketones, Acidic and alkaline hydrolysis of esters; Reactions: Hell-Volhard Zelinsky reaction,

Carboxylic acid derivatives (aliphatic): Preparation: Acid chlorides, anhydrides, esters and amides from acids and their interconversion, Claisen condensation. Reactions: Relative reactivities of acid derivatives towards nucleophiles, Reformatsky reaction, Perkin condensation.

Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of ethyl acetoacetate

**Unit 2: Amines (aliphatic & aromatic) and Diazonium Salts (Hours:10)**

Amines

Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hoffmann bromamide reaction. Reactions: Hoffmann *vs* Saytzeff elimination, carbylamine test, Hinsberg test, reaction with $HNO_2$, Schotten-Baumann reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation; basicity of amines.

Diazonium salt

Preparation: from aromatic amines; Reactions: conversion to benzene, phenol and dyes.

**Unit 3: Heterocyclic Compounds (Hours: 7)**

Introduction, classification, structure, nomenclature and uses. Preparation and properties of the following heterocyclic compounds with reference to electrophilic and nucleophilic substitution: furan, pyrrole, thiophene, and pyridine.

**Practical Component: Credits: 02**

**(Laboratory periods: 60)**

1. Systematic qualitative analysis and preparation of suitable crystalline derivative (carboxylic acids, carbonyl, alcohols, phenols, amines (1°, 2°, 3°) and amides).
2. Preparation:
   a. Acetylation of Aniline and Phenols.
   b. Benzoylation of Aniline and phenols

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.

**References:**

**Theory:**


1. Morrison, R. N.; Boyd, R. N. **Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. **Organic Chemistry** (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson

Education).

3. Ahluwalia, V.K.; Bhagat, P.; Aggarwal, R.; Chandra, R. (2005), **Intermediate for Organic Synthesis**, I.K. International.
4. Solomons, T. W. G.; Fryhle, C. B. ; Snyder, S. A. (2016), **Organic Chemistry**, 12$^{th}$ Ed., Wiley.

**Practical:**

1. Ahluwalia, V.K.; Dhingra, S.; Gulati, A. (2005), **College Practical Chemistry**, University Press (India) Ltd.
2. Ahluwalia, V.K.; Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
3. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.
4. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume II**, I K International Publishing House Pvt. Ltd., New Delhi.
5. Vogel, A.I. (1972), **Textbook of Practical Organic Chemistry**, Prentice-Hall.
6. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989), **Vogel's Textbook of Quantitative Chemical Analysis**, John Wiley and Sons.

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

## BSC. (PHYSICAL SCIENCES)- CHEMISTRY COMPONENT
## SEMESTER - V

### DISCIPLINE SPECIFIC CORE COURSE CHEM-DSC -13: Chemistry- V: Coordination Chemistry and Organometallics

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 | | |
| **Coordination Chemistry and Organometallics DSC-13: Chemistry- V** | **04** | **02** | **-** | **02** | **Class 12th with Physics, Chemistry, Mathematics** | |

### Learning Objectives

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

- To develop basic understanding of coordination chemistry and organometallics which are of immense importance to biological systems, qualitative quantitative analysis, catalysis, medicines, paints and pigments etc.
- The students learn nomenclature, isomerism and bonding in coordination compounds with special emphasis on important coordination compounds in the biological system.
- To understand classification of organometallic compounds, the concept of hapticity and the 18-electron rule governing the stability of a wide variety of organometallic species with special emphasis on metal carbonyls.

### Learning outcomes

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

- Understand terms: ligand, denticity of ligands, chelate, coordination number.
- Systematically name coordination compounds.
- Discuss the various types of isomerism possible in Octahedral and Tetrahedral coordination compounds.
- Use Valence Bond Theory to predict the structure and magnetic behaviour of metal complexes and understand the terms inner and outer orbital complexes.
- Explain the meaning of the terms $\Delta o.$, $\Delta t$, pairing energy, CFSE, high spin and low spin and how CFSE affects thermodynamic properties like lattice enthalpy and hydration enthalpy.

- Explain magnetic properties and colour of complexes on basis of Crystal Field Theory
- Apply 18-electron rule to rationalize the stability of metal carbonyls and related species.
- Learn how IR data can be used to understand extent of back bonding in metal carbonyls.

## Syllabus

**Unit 1: Introduction to Coordination compounds (Hours: 6)**

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

**Unit 2: Bonding in Coordination Compounds (Hours: 14)**

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

Crystal Field Theory: Splitting of d orbitals in octahedral symmetry. Crystal field effects for weak and strong fields, Crystal field stabilization energy (CFSE), concept of pairing energy, Factors affecting the magnitude of $\Delta$, Spectrochemical series, Splitting of d orbitals in tetrahedral symmetry, Comparison of CFSE for octahedral and tetrahedral fields, tetragonal distortion of octahedral geometry, Jahn-Teller distortion

**Unit 3: Organometallic Chemistry (Hours: 10)**

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

**Practical Component Credits:02**

**(Laboratory periods:60)**

1. Estimation of $Mg^{2+}$ by direct complexometric titrations using EDTA.
2. Estimation of $Zn^{2+}$ by direct complexometric titrations using EDTA.
3. Estimation of $Ca^{2+}$ by direct complexometric titrations using EDTA.
4. Estimation of total hardness of a given sample of water by complexometric titration.
5. Determination of the composition of the $Fe^{3+}$ - salicylic acid complex / $Fe^{2+}$-1, 10-phenanthroline complex in solution by Job's method.

6. Determination of the composition of the $Fe^{3+}$ - salicylic acid complex / $Fe^{2+}$-1,10-phenanthroline complex in solution by mole ratio method
7. Preparation of the following inorganic compounds:
   a). Tetraamminecopper(II) sulphate
   b). Potassium trioxalatoferrate(III) trihydrate
   c). Chrome alum
   d). *Cis*- and *trans*-Potassium diaquadioxalatochromate(III)
8. Any suitable experiment (other than the listed ones) based upon complexation 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. Cotton, F.A.; Wilkinson, G.; Gaus, P.L. **Basic Inorganic Chemistry**, 3rd Edition, Wiley India.
5. Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994), **Concepts and Models of Inorganic Chemistry**, John Wiley & Sons.
6. Greenwood, N.N.; Earnshaw, A. (1997), **Chemistry of the Elements**, 2nd Edition, Elsevier.
7. Lee, J.D.; (2010), **Concise Inorganic Chemistry**, Wiley India.
8. Sodhi G.S., **Principles of Inorganic Chemistry**, 3rd Edition, Viva Books India.


**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. Marr, G.; Rockett, B.W. (1972), **Practical Inorganic Chemistry**, Van Nostrand Reinhold.
3. Dua A, Manav N, **Practical Inorganic Chemistry,** (2017), Manakin Press.


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

## DISCIPLINE SPECIFIC CORE COURSES

**Semester – VII**

**DSC-I**

| Course title & Code | Credits | Credit distribution of the course | | | Eligibility criteria | Pre-requisite of the course (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical / Practice | | |
| **Advanced Inorganic & Organic Spectroscopy, Quantum Chemistry and Molecular Symmetry** (DSC-I) | **04** | **03** | — | **01** | Class 12th With Physics, Chemistry, Mathematics | -- |

### Inorganic Chemistry

**Learning Objectives**

The course is designed to provide the fundamental understanding of the principle of operation and interpretation of spectra of inorganic compounds for their structural characterization relevant to real world application.

**Learning Outcomes**

The students will learn to:

1. To analyze and interpret experimental data collected of inorganic materials using different spectroscopic techniques
2. To be able to learn and analyze the theory and principle of mass spectroscopy, various ionization techniques involved and different types of detectors used and to implement the theory to interpret the mass spectra.

**SYLLABUSOFDSC-1**

**Unit-1. Spectroscopy for Inorganic Materials**

ATR-IR, and Solid state or multinuclear NMR Spectroscopy of inorganic materials: Basics and applications of IR spectra in inorganic materials, total internal reflectance of inorganic materials, diffuse reflectance spectroscopy (DRS), Kubelka-Munk equation. $^{1}H$, $^{13}C$ NMR spectra of metal complexes, dipolar and contact shifts. Basics of Magic angle spinning NMR spectroscopy (MAS NMR).Example of solid-state NMR with $^{10}B$, $^{11}B$, $^{17}O$, $^{19}F$, $^{27}Al$, $^{29}Si$, $^{31}P$nuclei.(10 Lectures)

**Unit–2:Basics of Mass Spectrometry**

Mass spectrometry: Experimental arrangements, Ion sources, Mass analysers and detectors, Data analysis, Molecular ions, Fragmentation, Ion reactions, combined mass spectrometry methods, Tandem mass spectrometry (MS/MS), Chromatography-coupled mass spectrometry.(05 Lectures)

**Practical:**

1. Synthesis of substituted ferrocene and its mass-spectrometry analysis.
2. Synthesis of substituted Metal acetylacetonateand its mass-spectrometry analysis.
3. ATR-IR, NMR analysis of metal complexes acetylacetonate complexes of Iron, Manganese and Copper.

**Recommended Texts:**


1. Banwell, C.N.; McCash, E.M. (2006), Fundamentals of Molecular Spectroscopy, Tata McGraw- Hill.
2. Springsteen, A. (1998), Reflectance Spectroscopy: an overview of classification and techniques. In Applied Spectroscopy; Workman, J., Springsteen, A., Eds.; Academic Press 193–224. DOI: 10.1016/B978-012764070-9/50008-1.
3. Fitzgerald, J.J. and DePaul, S. M. (1999), Solid-State NMR Spectroscopy of Inorganic Materials: An Overview, 2-133, DOI: 10.1021/bk-1999-0717.ch001.
4. Brevard, C. and Granger, P. Handbook of high resolution multinuclear NMR, A Wiley publisher, 1981 and Brevard, C. The multinuclear approach to NMR spectroscopy, Springer Netherlands, 1983.
5. Nielsen, NielsChr, Strassø, Lasse A, and Nielsen, Anders B. Solid state NMR, Springer-Verlag Berlin Heidelberg, 2012.
6. D. W. Rankin, N. Mitzel, and C. Morrison, Structural methods in molecular inorganic chemistry. John Wiley & Sons, 2013.
7. E. A. V. Ebsworth, D. W. Rankin, and S. Cradock, Structural methods in inorganic chemistry. Blackwell Scientific Publications, Oxford, 1987.
8. William Henderson and J. Scott McIndoe, Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds: Tools – Techniques – Tips, John Wiley and Sons, Ltd, 2005, ISBN 0-470-85015-9
9. J.M. Modern spectroscopy, Hollas, 4th edition John Wiley and sons Ltd., 2004.

# Organic Chemistry

***Objectives:***Understanding spectroscopic techniques and their application in the structural elucidation of organic molecules.
***Course Outcomes:***The students will acquire knowledge of solving structural problems based on UV-VIS, IR, $^{1}$HNMR, $^{13}$CNMR, and Mass spectral data.

***Course/Learning Outcomes:***Students will gain an understanding of the basic principles of NMR spectroscopy, such as chemical shift, coupling constant, and anisotropy, and describe how they are affected by molecular structure, and identify organic compounds by analysis and interpretation of spectral data.

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***Theory Course Content:*** ***Credit 1 (15Lectures)***

Recapitulation of the Spectroscopic Techniques (UV- VIS, IR, and $^{1}$HNMR)**(2 Lectures)**

***13-CNMR and 2D NMR Spectroscopy:*** Resolution and multiplicity of $^{13}$C NMR, $^{1}$H-decoupling, noise decoupling, broadband decoupling; Deuterium, fluorine, and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR. DEPT and general introduction about 2D NMR.(**5 Lectures)**

***MASS:*** Theory, Fourier transform mass spectrometry instrumentation (FTMS); Unit mass and molecular ions; Important terms singly, doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity; Recognition of $M^{+}$ ion peak; Nitrogen rule; Rule of 13; Ionization methods (EI and ESI). General fragmentation rules: McLafferty rearrangement, ortho effect. **(4 Lectures)**

***ESR:*** Basic Principles and applications for organic Compounds **(2 Lectures)**

Structure elucidation of organic compounds using UV, IR, NMR, and Mass Spectra.
**(2 Lectures)**

***Recommended Reference and Textbooks:***


**1.** Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (**1991**).
**2.** Silverstein, R. M., Bassler, G. C. & Morrill, T. C. Spectroscopic Identification of Organic Compounds. John Wiley & Sons (**1981**).
**3.** Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. Introduction to Spectroscopy. Cengage Learning (**2014**).
**4.** Organic Structures from spectra; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., **2007**

## PRACTICALS

***Course Outcome:*** The students will acquire knowledge of:

1. Safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents.
2. Synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization.

| ***List of Practical's*** | ***Credit 1/3*** |
|---|---|

***(Spectra to be provided wherever required)***

1. Diels-Alder reaction between maleic anhydride and anthracene and identification of the product using IR and NMR Spectroscopy.
2. Knoevenagel condensation between aromatic aldehydes (benzaldehyde/*p*-nitrobenzaldehyde) and active methylene compounds (malononitrile/ethylcyanoacetate/diethylmalonate) and identification of the product using IR and NMR Spectroscopy.
3. Differentiate between maleic and fumaric acid solutions by UV spectroscopy.
4. Determination of the effect of pH on absorbance maximum (UV-Vis spectra) of the organic compounds. (Aniline, Benzoic acid, phenol etc.)
5. Demonstration of the separation of the mixture of *p*-nitrophenol and *o*-nitrophenol by columnchromatography and their characterization bymelting point and spectroscopic techniques.

***Recommended Reference and Textbooks:***


1. Vogel, A. I. (**2012**). Quantitative Organic Analysis, Part 3, Pearson Education.
2. Mann, F. G., Saunders, B.C. (**2009**), Practical Organic Chemistry, Pearson Education.
3. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (**2012**), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
4. Ahluwalia, V.K., Dhingra, S. (**2004**), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
5. Morrill, L. A., Kammeyer, J. K., & Garg, N. K. (**2017**). Spectroscopy 101: A practical introduction to spectroscopy and analysis for undergraduate organic chemistry laboratories.*J. Chem. Educ.*94(10), 1584-1586.

# Physical Chemistry

**Course Objectives:**

- To introduce fundamental concepts of quantum mechanics, including vector spaces, operator algebra, angular momentum, spin, and the application of these concepts to atomic and molecular systems.
- To develop a quantitative understanding of Dirac notation, commutation relations, the Heisenberg Uncertainty Principle, and spin eigenfunctions.
- To provide a foundational understanding of molecular symmetry through symmetry elements, point groups, and character tables.
- To apply group theory to interpret spectroscopic data, derive selection rules, and understand molecular vibrations in infrared and Raman spectroscopy.

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

- Understand the basic concepts and quantitative aspects of chemical phenomena, which require knowledge of both quantum chemistry and mathematics.
- Apply relevant mathematical methods essential for solving problems in quantum chemistry.
- Interpret symmetry elements and operations in molecules using the principles of group theory.
- Predict spectroscopic transitions using symmetry considerations and selection rules.
- Demonstrate an integrated understanding of how quantum chemistry and group theory together contribute to the interpretation of molecular spectroscopy.

**Theory Course Contents:** **Credit 1 (15 lectures)**

**Unit I: Quantum Chemistry (7 lectures)**

Introduction to vector spaces (Particle in 1-D box), Dirac's Bra-ket notation, Turn-over rule, Commutation of operators Heisenberg's Uncertainty principle (derivation and physical significance), Angular momentum: definitions, creation and annihilation operators; spherical harmonics, Spin operators and eigenfunctions; two-electron systems (qualitative).

**Unit II: Molecular Symmetry (8 lectures)**

Symmetry elements and operations; Point groups ($BF_3$, $NH_3$, $H_2O$), Classes,reducible and irreducible representations, Similarity transformation, Character table&Great Orthogonality Theorem (without proof)), Transition moment integrals, Selection Rules, IR and Raman activity: Group theoretical approach, examples predicting vibrational activity using character tables.

**Recommended Texts/References:**


1. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).
2. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).
3. Mortimer, R. G. Mathematics for Physical Chemistry 2nd Ed. Elsevier (2005).
4. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).
5. Atkins, P. W. &Friedman, R.S.,Molecular Quantum Mechanics 3rd Ed., Oxford University Press (2004).

6. Kakkar R., *Atomic and Molecular Spectroscopy*, Cambridge University Press, (2015).
7. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
8. Bakhshi, A. K., and Thakral P., Quantum Chemistry Simplified, Vidyavani Foundation, New Delhi, ISBN: 9788196225107 (2023).
9. Cotton, F. A. Chemical Applications of Group Theory Wiley Interscience: N.Y (1990).
10. Bishop, D. M. Group Theory and Chemistry, Clarendon Press: Oxford, U.K. (1973)

**Supplementary readings**

11. Quantum Chemistry and Group Theory, MCH-018, IGNOU Self Learning Material, egyankosh, Indira Gandhi National Open University (2025) https://egyankosh.ac.in/handle/123456789/107771
12. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley (2004)
13. Rakshit, S. C.; Atomic & Molecular Symmetry Groups and Chemistry, CRC Press, Taylor and Francis Group.

**Laboratory Exercises (Practical) (atleast four):** **Credit 1/3**

1. Determine the specific reaction rate of the potassium persulphate-iodide reaction by the Initial Rate Method.
2. Titrate a moderately strong acid (Salicylic/Mandelic acid) by the (a) salt-line method (b) double alkali method.
3. Titrate a tribasic acid (phosphoric acid) against NaOH potentiometrically.
4. Plotting of atomic orbitals (Spherical Harmonics S(θ) versus θ using polar graph paper. Student will be provided with the *p*-, *d*- and *f*- functions.
5. Plotting of $\psi_n(x)$, and $|\psi_n(x)|^2$ for wavefunctions of 1D harmonic oscillator in different energy levels within the domain of $x$, $-\infty < x < +\infty$.
6. Calculate the bond length of conjugated dye molecules (i.e., cyanine/β-carotene) using particle in 1D box model.
7. Simulated IR Spectra: assign bands using symmetry and selection rules.

**Recommended Texts/References:**

1. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).
2. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
3. Kapoor, K.L., A Textbook of Physical Chemistry, Vol. IV, fifth Edition, McGraw Hill Education.
4. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).

**Semester – VIII**

**DSC-II**

| Course title &Code | Credits | Credit distribution of the course | | | Eligibility criteria | Pre-requisiteof the course (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical / Practice | | |
| **Advanced Bioinorganic Chemistry, Application of Reagents in Organic Synthesis, Statistical Thermodynamics and Applications** | **04** | **03** | — | **01** | Class 12th With Physics, Chemistry, Mathematics | -- |

## Inorganic Chemistry

**Unit I: Metals in Biological System**

Biominerals and biomineralization, Detailed study of biocatalyst in the metabolism of Hydrogen, carbon, and sulfur, Biological actions of manganese, cobalt and nickel ions, Metal ions in brain and medicine, Homeostasis of Metals, Potassium-Dependent Molecules, Inorganic Nanoparticles in Wound Healing and Drug Delivery (5 Lectures)

**Unit II: Inorganic Materials for Biomedical Applications**

Natural Bone Structure and Composition, Calcium Phosphate Ceramics (e.g., hydroxyapatite, tricalcium phosphate), Metal Implants (e.g., titanium, stainless steel), Natural Tooth Structure and Composition (enamel, dentin), Dental Ceramics (e.g., zirconia, alumina), 3D Bioprinting.
(10 Lectures)

**Course Objective:**

This course delves into the fascinating intersection of bio-inorganic metals and their crucial roles in living systems. The detailed investigation of bio-inorganic chemistry of essential elements towards biomedical applications.

**Course Outcome:**

Upon successful completion of this course, the students will be able to:

Understand the advance application of bio-inorganic metals.
Explore the structure and properties of inorganic materials used in biomedical applications.
Investigate the biocompatibility and bioactivity of inorganic biomaterials.
Discuss current research and future directions of bio-inorganic chemistry.

**Practical Components:**

1. Synthesis and characterization of calcium phosphate ceramics spectrophotometrically /any other method.
2. Analyzing the composition of Bio materials(Stainless steel, hydroxyapatite)
3. Fabrication of a simple Bio-hydrogel (Polyvinyl alcoholhydrogel, polysaccharide hydrogel, cellulose,starch)
4. Preparation of Zirconia($ZrO_2$).
5. Preparation and characterisation of transition metal complexes of riboflavin using commercially available Vitamin B2 supplements

**References:**


1. Bio-coordination Chemistry, D E Fenton, OUP, 2002
2. Principles of Bioinorganic Chemistry, S J Lippard and, J M Berg, USB, California, 1994
3. Biological Inorganic Chemistry, R.R Crichton, Elsevier, 2012
4. Y. Bar-Cohen, Biomimetics: Biologically Inspired Technologies, Taylor & Francis CRC Press, Boca Raton, FL, 2006.
5. R.L. Reis, S. Weiner, Learning from Nature How to Design New Implantable Biomaterials, Kluwer Academic Publishers, New York, 2005.
6. P. Behrens, E. Bäuerlein, Handbook of Biomineralization: Biomimetic and Bioinspired Chemistry, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007.
7. H. Lowenstam, S. Weiner, On Biomineralization, Oxford University Press, New York, 1989.
8. S. Mann, Biomineralization: Principles and Concepts in Bioinorganic Materials Chemistry, Oxford University Press, Oxford, New York, 2001.
9. E. Bäuerlein, Biomineralization: Progress in Biology, Molecular Biology and Application, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.
10. E. Bäuerlein, Handbook of Biomineralization: Biological Aspects and Structure Formation, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007.
    F.E. Round, R.M. Crawford, D.G. Mann, The Diatoms: Biology and Morphology of the Genera, Cambridge University Press, Cambridge, 1990.


## Organic Chemistry

***Objectives:***Tofacilitate chemical transformations by providing the necessary conditions and catalysis.

***Course Outcome:***At the completion of this course, the students should be able to:

i) Understand various reducing agents, oxidizing agents, and their applications in organic synthesis.

ii) Understand the conversion of specific functional groups without affecting othersand maximize yields and selectivity for the desired products.

***Theory Course Content*** ***1 Credit (15 lectures)***

i. Synthesis and applications of BuLi, Grignard, organoaluminium, and organozinc reagents. **(3 Lectures)**

ii. ***Reagents in Organic Synthesis***: Triacetoxyborohydride, Lead Acetate, Phenyliodine (III) diacetate (PIDA), DCC, Tamao-Fleming Oxidation; Dimethyldioxirane (DMDO) Oxidation; DMSO (Barton modification &Swern Oxidation); Oxidation of organic compounds using thallium nitrate, selenium dioxide, phase transfer catalyst, crown ethers, $KMnO_4$, PCC, $OsO_4$, $CrO_3$, $K_2Cr_2O_7$. **(10 Lectures)**

ii. Applications of hydroboration (reductions, oxidations, and carbonylation): Diborane, 9-BBN. **(2 Lectures)**

***Recommended Reference and Textbooks:***


1. Carruthers, W. Modern Methods of Organic Synthesis. Cambridge University Press (**1996**).
2. Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (**2004**).
3. Jonathan Clayden, Nick Greeves, Stuart Warren. Organic Chemistry. Oxford. (**2000**)


## PRACTICALS

***Course Outcome:*** The students will acquire knowledge of:

1. Safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents.
2. Characterization by physical and spectroscopic techniques.

***List of Practical's*** ***Credit: 1/3***

Identification of the product based on Melting point and spectroscopic techniques (IR, $^1$HNMR, and $^{13}$C NMR spectroscopy, data to be provided).

1. Synthesis of 1,2,3,4-tetrahydrocarbazole from cyclohexanone.
2. Reduction of *p*-nitrobenzaldehyde using suitable reagents. ($NaBH_4$/Sn-HCl)
3. Synthesis of 2,3-diphenylquinoxaline from benzil and *ortho*-phenylenediamine.
4. Oxidation of Aryl Aldehydes into Ester by $I_2$ and Alcohols.

***Recommended Reference and Textbooks:***


1. Ahluwalia, V. K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.

2. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
3. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
4. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi

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## Physical Chemistry

**Course Objectives:**

- To provide a brief foundational understanding of the core principles of classical and quantum statistical mechanics.
- To explore the connection between macroscopic thermodynamics and microscopic quantum mechanics using various statistical ensembles.
- To introduce the Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics with a brief, qualitative understanding and focus on their applications.
- To enable students to apply statistical concepts in key areas such as the standard model for macromolecular systems, chemical kinetics, and chemical equilibrium.

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

- Understand the fundamental principles of statistical mechanics, including how they link microscopic behaviour to macroscopic properties of systems.
- Apply the Boltzmann distribution, Bose-Einstein statistics, and Fermi-Dirac statistics to various physical and chemical systems.
- Utilize partition functions to analyze and solve problems related to the thermodynamic properties of systems.
- Explore the application of statistical mechanics to key areas such as chemical kinetics, chemical equilibrium, and random walk models in macromolecular systems.

**Course Contents (Theory):** **Credit 1 (15 lectures)**

**Unit I- Statistical Thermodynamics (8 lectures)**
Microstates, Configurations, coin tosses, rolling of dices, spin systems (in the absence of magnetic field),Thermodynamic probability, Stirling's approximation, Concepts of ensembles (Microcanonical and Canonical), Characteristic thermodynamic functions, Translational partition function (quantitative), Rotational and vibrational partition functions (qualitative), Maxwell-Boltzmann distribution, Bose-Einstein, and Fermi-Dirac Statistics (Qualitative).

**Unit II-Applications (7 lectures)**
Conventional transition state theory derived from partition functions, Equilibrium constants in terms of partition function: gas-phase reactions ($K_p$),isotope effects.
1-D random walk model, Number and weight average molecular weight, polydispersity index.

**Recommended Texts/References:**


1. McQuarrie, D. A. *Statistical Mechanics,* Viva Books Pvt. Ltd.: New Delhi (2003).
2. L. D. Landau and E. M. Lifshitz, Statistical Mechanics, Part I, Butterworth-Heinemann, 3rd ed. (2005).
3. Bagchi B. *Statistical Mechanics for Chemistry and Material Science,* CRC Press (2018).
4. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).
5. Billmeyer, F. W. *Textbook of Polymer Science* 3rd Ed. Wiley-Interscience: New York (1984).
6. Pathria, R.K.; and Beale, P. D.;Statistical Mechanics, Fourth Edition, Elsevier, Academic press.
7. Huang, K., Statistical Mechanics, 2nd Ed., John Wley& Sons, New York (2000)


**Laboratory Exercises (Practical) (atleast four):** **Credit 1/3**

1. Study the kinetics of the iodination of acetone in the presence of acid by the *Initial Rate Method*.
2. Titrate a tribasic acid (phosphoric acid) against NaOH and $Ba(OH)_2$ conductometrically.
3. Find the composition of the zinc ferrocyanide complex by potentiometric titration.
4. Statistical Treatment of Error Analysis (Null Hypothesis, T-test, F-test, Q-test (criteria for reject of hypothesis) Statistical analysis of laboratory data.
5. Determination of standard deviation, mean and maximum absolute errors, root-mean-square deviation (error) and Correlation coefficient of linear straight-line plot.

**Recommended Texts/References:**


1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
2. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).
3. Skoog, D. A.; Holler, F. J.; Crouch, S. R. Principles of Instrumental Analysis, Brooks/Cole Pub Co; 7th edition (1 January 2017).
4. Skoog, D. A.; West, D. M.; Holler, F. J.; Crouch, S. R. Fundamentals of Analytical Chemistry, Publisher: Holt, Rinehart & Winston of Canada Ltd; International 2 Revised ed edition (1 February 1988).

**DISCIPLINE SPECIFIC ELECTIVE COURSES**

**SEMESTER – VII**

**INORGANIC CHEMISTRY**

## DISCIPLINESPECIFICELECTIVECOURSE-1(DSE-1):Inorganic Main Group Clusters-Basics and Applications

### CREDITDISTRIBUTION,ELIGIBILITYANDPRE-REQUISITESOFTHE COURSE

| Coursetitle & Code | Credits | Creditdistributionofthe course | | | Eligibility criteria | Pre-requisite ofthecourse (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| **Main Group Clusters-Basics and Applications (DSE-1)** | **04** | **02** | **--** | **02** | Class12$^{th}$ with Physics, Chemistry | **--** |

**Objectives:**
To introduce the basic concepts of clusters.To gather a good understanding of the chemistry and various aspects of main group cluster compounds with respect to synthesis, structure and properties.

**Learning Outcomes:**On completion of the course, the students will be able to:

1. Ensures the students understand the concepts and the properties of clusters.
2. Acquire knowledge of cluster compounds and explain structure-property, electron counts, and surface analogies of cluster compounds.
3. Identify the structure and bonding aspects of main group clusters.
4. Identify the different types of main group cluster reactions and apply the above concepts to explain reactivity of the clusters.

### SYLLABUSOFDSE-1

Introduction to molecular clusters - Clusters in elemental states, cluster classification, skeletal electron (Elm) counting.
Main-group clusters: Geometric and electronic structure, three-, four- and higher connect clusters, the *closo-, nido-, arachno-hypho-, klado-,*borane structural paradigm, Wade-Mingos and Jemmis electron counting rules,Lipscomb topological diagrams, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity.Heteroboranes,boron-carbides and metal-borides.Illustrative examples from recent literature.(30 Lectures)

**Keywords:** Clusters, skeletal electron count, boranes, synthesis, reactivity.

**Teaching Learning Process:**
Lectures, ICT enabled teaching, presentations by students, group discussion and quiz will be the part of teaching learning process.

**Assessment Methods:**
● Presentations by Individual Student/ Group of Students
● Class Tests at Periodic Intervals.
● Written assignment(s)
● End semester University Theory Examination

**Practical**

1. Determination of Boron colorimetrically.
2. Preparation of borax/ boric acid.
3. Synthesis of zinc borate from zinc oxide and boric acid and their analysis using various instrumentation techniques: IR, UV, TGA, and DSC. Thermal decomposition of borax and its structural characteristics using XRD, FTIR.
4. Qualitative analysis of cobalt, nickel, copper etc. using borax (borax bead test).
5. Other new novel synthesis reported in literature from time to time
6. Syntheses and characterisation of zinc(II)acetylacetonate and tin(II)acetylacetonate complexes

**Text Books:--**


1. M. P. Mingos and D. J. Wales; Introduction to Cluster Chemistry, Prentice Hall, 1990.
2. N. Greenwood and E. A. Earnshaw; Chemistry of elements, Second Edition, Butterworth-Heinemann, 1997.
3. P. Fehlner, J. F. Halet and J-Y. Saillard; Molecular Clusters: A Bridge to solid-state Chemistry, Cambridge University press, 2007.
4. B. D. Gupta and A. J. Elias; Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, Universities Press (India), 2010.
5. M. P. Mingos, Essential Trends in Inorganic Chemistry, Oxford, University Press, 1998.
6. C. E. Housecroft, Metal-Metal Bonded Carbonyl Dimers and Clusters, Oxford Chemistry Primers (44), Oxford, University Press, 1996.


**Reference Books:**


1. F. Holleman and E. Wifrg, Inorganic Chemistry, Academic Press, New York, 1995.
2. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn, John Wiley & Sons, Inc, New York, 1999.

3. G. Wulfsberg, Inorganic Chemistry, Viva Books Pvt Ltd, New Delhi, 2001.
4. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.
5. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Shriver & Atkins Inorganic Chemistry,
4th Edn, Oxford, 2006.
6. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Inorgnic Chemistry: Principles of Structures and Reactivity, 4th Edn, Pearson, New Delhi, 2006.
7. R. Xu, W. Pang and Q. Huo (Eds), Modern Inorganic Synthetic Chemistry, Elsevier, New York, 2011.
8. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd Edn, Pearson, New Delhi, 2009.
9. J. R. Anderson and M. Boudart (Eds), Catalysis: Science and Technology, Springer, London, 2012.
10. P. Powell, Principles of Organometallic Chemistry, 2nd Edn, Chapman and Hall, London, 1988.
11. G. O. Spessard and G. L. Miessler, Organometallic Chemistry, International 2nd Edn, Oxford University Press, Oxford, 2010.
12. D. F. Shriver, H. D. Kaesz and R. D. Adams (Eds), The Chemistry of Metal Cluster Complexes, VCH, New York, 1990.
13. K. J. Klabunde, Free Atoms, Clusters and Nanoscale Particles, Academic Press, New York, 1994.
14. D. M. P. Mingos (Ed.), Structural and Electronic Paradigms in Cluster Chemistry, Springer, Berlin, 1997.
15. P. Braunstein, L. A. Oro and P. R. Raithby (Eds), Metal Clusters in Chemistry, Wiley-VCH, Weinheim, 1999.
16. M. Driess and H. Noth (Eds), Molecular Clusters of the Main Group Elements, Wiley-VCH, Weinheim, 2004.
17. C. E. Housecraft and A. G. Sharpe, Inorganic Chemistry, 3rd Edn, Pearson Education Ltd, Essex, England, 2008.
18. F. Wells, Structural Inorganic Chemistry, 5th Edn, Oxford University Press, Oxford, 1984.

## DISCIPLINESPECIFICELECTIVECOURSE-2(DSE-2):

## Advanced Coordination Chemistry

### CREDITDISTRIBUTION,ELIGIBILITYANDPRE-REQUISITESOFTHE COURSE

| Coursetitle & Code | Credits | Creditdistributionofthe course | | | Eligibility criteria | Pre-requisite ofthecourse (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| **Advanced Coordination Chemistry (DSE-2)** | **04** | **02** | **--** | **02** | Class12th with Physics, Chemistry, Mathematics | **--** |

**Objectives:**

- To introduce the basic concepts of coordination polymers and porous and cavity containing structures.
- To gather a good understanding of the chemistry, principles, design and synthesis of coordination polymers like metal-organic frameworks, coordination clustersalong with exploring their structures, properties and applications.

**Learning Outcomes:**

On completion of the course, the students will be able to:

- Have a strong foundation in understanding the basic concepts and properties of coordination polymers and porous and cavity containing systems.
- Gain an understanding of the different types of structures (single metal-noded, metal cluster-noded, pillared layer nets) of coordination polymers.
- Acquire knowledge on synthesis methods and how reaction conditions in synthesis can be used to design targeted coordination polymers.
- Acquire knowledge on the different types of structures of coordination polymers, e.g. MOFs, coordination clusters, etc and applications in catalysis and hydrogen storage.
- Learn about the design and morphology of self-assembling coordination compounds using suitable examples.

### SYLLABUSOFDSE-2

Coordination polymers, assembly, single metal-noded nets, metal cluster-noded nets, pillared layer nets, and structural modulation by reaction conditions, including in situ metal/ligand reactions.

Coordination Polymers: Metal-Organic Frameworks and Other Terminology , 0D Coordination Clusters , 1D, 2D and 3D Structures , Magnetism , Negative Thermal Expansion , Interpenetrated Structures , Porous and Cavity-Containing Structures, Catalysis by MOFs , Hydrogen Storage by MOFs,

Self-Assembling Coordination Compounds: Design and Notation, Supramolecular Cube, Molecular Squares and Boxes, Self-Assembly of Metal Arrays (30 Lectures)

**Keywords:**
Coordination polymers, metal-organic frameworks, self-assembly, catalysis, hydrogen storage

**Teaching Learning Process:**
Lectures, ICT enabled teaching, presentations by students, group discussion and quiz will be the part of the teaching learning process.

**Assessment Methods:**
● Presentations by Individual Student/ Group of Students
● Class Tests at Periodic Intervals.
● Written assignment(s)
● End semester University Theory Examination

**Practical:**

1. Preparation of zeolite A and removal of Mg and Ca ions from water samples quantitatively using prepared zeolite A.
2. Estimation of $MnO_2$ in pyrolusite.
3. Preparation and characterization of following the following complexes/organometallic compound including their structural elucidation by the available physical methods. (Element analysis, molecular weight determination, conductance and magnetic measurement and special studies):
    - Synthesizing a nickel-citric acid coordination polymer using nickel nitrate, citric acid, and dimethylformamide (DMF) under solvothermal conditions.
    - Synthesizing Cu(II) coordination Polymers with 4,4-bipyridine.
    - Synthesis of *cis* and *trans* isomers of bis(glycinato) copper(II) monohydratye.
    - Synthesis of Cu acetate complex
4. Solid State synthesis-
    - Preparation of oxides and mixed oxides ($Mn_2O_3$, NiO, $Cu_2O$, $Fe_3O_4$, $ZnFe_2O_4$, $ZnMn_2O_4$, $CuMn_2O_4$ and $NiFe_2O_4$).
    - Preparation of Silica and Alumina by sol-Gel technique.
5. To study the electrical conductivity of ferrites, Magnetites, doped oxides and pure samples and determine band gap.

**Books for practical:**

1. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
2. Inorganic Experiments, J. DerckWoollins, VCH.
3. Practical Inorganic Chemistry, G. Marrand, B. W. Rockett, Van Nostrand.
4. A Text Book of Quantitative Inorganic Analysis, A. I.Vogel, Longoman.
5. EDTA Titrations. F. Laschka
6. Instrumental Methods of Analysis, Willard, Merit and Dean (CBS, Delhi).
7. Inorganic Synthesis, Jolly
8. Instrumental Methods of Chemical Analysis, YelriLalikov
9. Fundamental of Analytical Chemistry, Skoog D.A. and West D.M Holt Rinehart and Winston Inc.
10. Experimental Inorganic Chemistry, W. G. Palmer, Cambridge.
11. Solid state Chemistry, N. B. Hanney
12. Introduction to Thermal Analysis, Techniques and Applications, M.E.Brown, Springer
13. Preparation and Properties of solid state Materials, Wilcox, Vol.IandII, Dekker
14. The Structure and Properties of Materials Vol.IV, JohnWulff, Wiley Eastern.

**References:**


1. S.R. Batten, S.M. Neville, D.R. Turner, Coordination Polymers: Design, Analysis and Application, the Royal Society of Chemistry, Cambridge, UK, 2009.
a. A.F. Wells, Three-Dimensional Nets and Polyhedra, Wiley-Interscience, New York, 1977.
b. A.F. Wells, Further Studies of Three-dimensional Nets, ACA Monograph No.8, American Crystallographic Association, Knoxville, TN, 1979.
c. A. F. Wells, Structural Inorganic Chemistry, fifteenth ed., Oxford University Press, Oxford, 1984.
2. J. Weitkamp, L. Puppe, Catalysis and Zeolites: Fundamentals and Applications, Springer, 1999.
3. D.W. Breck, Zeolite Molecular Sieves: Structure, Chemistry, and Use, Wiley, New York, 1973.
4. J.W. Steed, J. L. Atwood, Supramolecular Chemistry Chapters 9 and 10. pp. 561-583 and 620-637, John Wiley & Sons Ltd, Second Edition (2e, 2009) ISBN: 9781119582519
5. R.M. Barrer, Hydrothermal Chemistry of Zeolites, Academic Press, London, 1982.
6. J. Cejka, H. van Bekkum, A. Corma, et al., Introduction to Zeolite Molecular Sieves third ed. (Studies in Surface Science and Catalysis, Vol. 168), Elsevier, 2007.
7. S.M. Auerbach, K.A. Carrado, P.K. Dutta, Handbook of Zeolite Science and Technology, CRC, 2003.
8. C.J. Brinker, G.W. Scherer, Sol-Gel Science, Academic Press, New York, 1990.

9. R. Szostak, Molecular Sieves: Principles of Synthesis and Identification, Blackie Academic & Professional, London, 1998.

# ORGANIC CHEMISTRY

## DISCIPLINE-SPECIFIC ELECTIVECOURSE-I (DSE-I)

### Title: Advanced Stereochemistry (DSE-I, 30 Lectures)

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

| Coursetitle &Code | Credits | Credit distribution | | | Eligibility criteria | Pre-requisite (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| AdvancedStereochemistry (DSE-I, 30 Lectures) | 04 | 02 | --- | 02 | Class 12$^{th}$with Physics,Chemistry, Mathematics | |

***Objectives:***To provide a comprehensive understanding of molecular symmetry, isomerism, and chirality, including their applications in organic reactions.

***Course Outcomes***:

1. Students will be expected to gain knowledge of the basic concept of chirality in molecules due to their spatial arrangement of atoms that leads to chiroptical properties.
2. The three-dimensional arrangement of atoms in a molecule can lead to distinct physical and chemical properties, particularly for stereoisomers.Understanding stereochemistry is crucial for designing effective drugs, predicting reaction outcomes, and developing new materials.
3. Stereochemistrysignificantly impacts drug action, biological processes, and chemical reactions, influencing factors like drug efficacy, selectivity, and even the rate of chemical reactions.

***Theory Course Content:*** ***Credit 2 (30Lectures)***

***Stereoisomerism:*** Chiral (stereogenic) centre, principle of axial and planar chirality; Stereochemistry and configurations of biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes, allenes, spiranes, alkylidine cycloalkanes, adamantanes, catenanes and helicity. **(15 Lectures)**

***Topicity and prostereoisomerism*:**Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres. **(5 Lectures)**

***Asymmetric induction:*** Cram's, Prelog's, and Felkin-Ahn model. **(3 Lectures)**

***Cyclostereoisomerism*:** Configurations, conformations and stability of cyclohexanes (di-, and tri-substituted), cyclohexenes, cyclohexanones, decalin. **(5 Lectures)**

Applications of ORD and CD to Stereochemical Problems (**2 Lectures**)

***Reference and Textbooks:***

**1.** Eliel, E. L. (2000), Stereochemistry of Carbon Compounds, Tata McGraw-Hill.

**2.** Nasipuri, D.(2018), Stereochemistry of Organic Compounds: Principles and Applications, 4th Edition, New Age International.

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# PRACTICALS

***Course Outcome:***

1. Understand the spatial arrangement and naming conventions of**E/Z and cis-trans stereoisomers**
2. Visualise chiral centres and identify enantiomers/diastereomers
3. Understand photo-induced isomerization
4. Resolution of enantiomers by formation of diastereomeric adducts

***List of Experiments*** ***2 Credit***

***(Any 10 practicals may be done depending upon the availability of resources.)***

1. E/Z and Cis-Trans Isomerism of 2,3-dimethyl-2-butene by ball and stick models
2. Identification of ChiralCentres and Diastereomers by ball and stick models
3. Bromination of cis and trans stilbene
4. Addition of Bromine to trans-Cinnamic Acid
5. Photoinduced isomerization of *cis*-Stilbene to *trans*-Stilbene and *vice versa*
6. Photocatalytic/ thermal isomerization of maleic acid to fumaric acid.[3]
7. Preparation of stilbene dibromide by bromination of *trans*-stilbene.
8. Determination of optical rotation of sucrose, glucose, and fructose using polarimetry and determiningtheir concentration.
9. Two-step synthesis of acetonide from benzil and analysis of its stereochemistry using NMR and IR spectroscopy
10. Determination of specific rotation of(R)-limonene and (S)-limonene using Polarimeter.
11. Preparation of hydroxybenzoin by pinacol coupling reaction: Investigating the Diastereoselectivity of Benzaldehyde Pinacol Coupling Mediated by Al-KOH in Aqueous Media: Affording *meso*- and dl-Hydrobenzoin.[4]
12. Proline-catalyzed aldol reaction of cyclohexanone with nitro-substituted benzaldehydes.[5]

***Recommended Reference and Textbooks:***

1. Microscale Organic Laboratory (Multistep and Multiscale Syntheses). By Dana W. Mayo, Ronald M. Pike, David C. Forbes.**2011**

2. Green Organic Chemistry: Strategies, Tools, and Laboratory Experiments, Kenneth M. Doxsee, James E. Hutchison. Thomson-Brooks/Cole, **2004**

3. The photochemical isomerization of maleic to fumaric acid: an undergraduate organic chemistry experiment. Albert J. Castro, Suzanne R. Ellenberger, and James P. Sluka. *J. Chem. Edu.***1983**,*60* (6), 521 (DOI: 10.1021/ed060p52)

4. Using $^{1}$H NMR Spectroscopy to Investigate the Diastereoselectivity of Benzaldehyde Pinacol Coupling Mediated by Al-KOH in Aqueous Media: An Undergraduate Lab Experiment Involving a Green Carbon–Carbon Bond-Forming Reaction Affording *meso*- and dl-Hydrobenzoins. Shahrokh Saba**;** Isabella Fante; James A. Cordero Jr.*J. Chem. Educ.* 2025, 102, 2, 847–851) doi.org/10.1021/acs.jchemed.4c01379

5. Proline-catalyzed asymmetric reactions. List, Benjamin. *Tetrahedron*. **2002**, 58 (28): 5573–5590. doi:10.1016/S0040-4020(02)00516-1

# DISCIPLINE-SPECIFIC ELECTIVE COURSE-II (DSE-II)

## Title: Reactive Intermediates of Organic Chemistry (DSE-II, 30 Lectures)

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

| Coursetitle &Code | Credits | Credit distribution | | | Eligibility criteria | Pre-requisite (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| ReactiveIntermediates of Organic Chemistry (DSE-II, 30 Lectures) | 04 | 02 | --- | 02 | Class 12$^{th}$with Physics,Chemistry, Mathematics | |

***Objectives:***To learn and understand the involvement of intermediates,their role in reaction mechanisms, predict their behavior, and apply this knowledge to organic synthesis. Also, to learn and understand the orbital interactions (Woodward-Hoffmann rules) in concerted reactions.

***Course Outcomes***:At the completion of this course, the students should be able to:

i. Understandthe structure-reactivity pattern of reactive intermediates involved in organic reactions.

iiWrite themechanism of organic reactions involving reactive intermediates and apply these reactions in organic synthesis

***Theory Course Content*** ***2 credit (30 Lectures)***

***Carbocations:***Difference between classical and non-classical carbocations.Introduction of neighboring group participation (NGP), ion-pairs, molecular rearrangements in acyclic, monocyclic, and bicyclic systems, stability and reactivity of bridgehead carbocations.

**(8 Lectures)**

***Carbanions:*** Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications. **(3 Lectures)**

***Carbenes:*** Structure of carbenes, generation of carbenes, addition and insertion reactions,rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylid by carbenoid decomposition. Examples of inter/intramolecular insertions.

**(7 Lectures)**

***Nitrenes:***Structure of nitrene, generation and reactions of nitrene and related electron-deficient nitrogen intermediates, Curtius, Hoffmann, Schmidt, Beckmann rearrangement reactions.

**(5 Lectures)**

***Ylides:***Chemistry of Phosphorus and Sulfur ylids – Wittig and related reactions, Peterson olefination. **(2 Lectures)**

***Radicals:*** Generation of radical intermediates and their addition to: i) on alkenes, alkynes (inter & intramolecular) for C-C bond formation and Baldwin's rules.ii) fragmentation and rearrangements. Name reactions involving radical intermediates, such as Barton deoxygenation and decarboxylation, McMurry coupling. **(5 Lectures)**

***Recommended Reference and Textbooks:***


**1.** A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5$^{th}$edition, Springer, New York, **2007**.

**2.** Carruthers and I. Coldham, Modern Methods of Organic Synthesis, First South Asian Edition 2005, Cambridge University Press.

**3.** March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley, **2007**.


## PRACTICALS

***Course Outcome:*** The students will acquire knowledge of:

**1.** Starting materials, functional groups, mechanism, and typical reaction conditions.

**2.** Characterisation by physical and spectroscopic techniques.

| ***List of Experiments*** | ***2 Credit*** |
|---|---|

**1.** Separation, purification, and identification of binary mixtures of organic compounds (neutral and acidic; neutral and basic) using chemical methodsand preparation of a suitable crystalline derivative for both the components. (Examples: (i) Benzoic acid/Any dicarboxylic acid and Naphthalene (ii)*p*-toludine/*p*-anisidine and Naphthalene)

**2.** **Two-step synthesis**

**2.1** ***Synthesis of triacetoxybenzene***

*Step 1:*Synthesis of *p*-benzoquinone from hydroquinone using $KBrO_3$ and

*Step 2:*Synthesis of Triacetoxybenzene from *p*-benzoquinone.

**2.2** ***Synthesis of p-acetamido benzene sulphonamide***

*Step 1:*Synthesis of *p*-Acetamido benzene sulfonyl chloride from acetanilide and

*Step 2:* Synthesis of *p*-Acetamido benzene sulphonamide from *p*-Acetamido benzene sulfonyl chloride.

***2.3*** ***Synthesis of benzopinacolone***

*Step 1:*Synthesis of benzopinacol from benzophenone

*Step 2:* Synthesis of benzopinacolone from benzopinacol *via* pinacol-pinacolone rearrangement.

***Recommended Reference and Textbooks:***


**1.** Vogel, A. I. (**2012**), Quantitative Organic Analysis, Part 3, Pearson Education.

**2.** Mann, F. G., Saunders, B.C. (**2009**), Practical Organic Chemistry, Pearson Education.

3. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (**2012**), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
4. Ahluwalia, V.K., Dhingra, S. (**2004**), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
5. Ahluwalia, V. K., Aggarwal, R. (**2004**), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
6. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
7. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi

## PHYSICAL CHEMISTRY

**DISCIPLINE SPECIFIC ELECTIVE COURSE-I (DSE-I):**

**Title: Advanced Molecular Spectroscopy and Applications (DSE-I, Semester-VII, 30 Lectures)**

| Course title & Code | Credits | Credit distribution of the course | | | Eligibility criteria | Pre-requisite of the course (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Advanced Molecular Spectroscopy and Applications (DSE-I, Semester-VII, 30 Lectures) | 04 | 02 | --- | 02 | Class 12th with Physics, Chemistry, Mathematics | --- |

**Course Objectives:**

- Introduce the principles of molecular spectroscopy across electronic, vibrational, rotational, and nuclear domains.
- Apply quantum mechanical concepts such as the Born–Oppenheimer approximation, Heisenberg's Uncertainty Principle, and time-dependent perturbation theory to spectroscopic transitions.
- Use symmetry and operator-based formalisms to derive selection rules.
- Analyze UV-Vis, fluorescence, Raman, Mössbauer, and CD spectroscopy.
- Explore applications in structure elucidation, dynamics, and single-molecule detection.

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

- Understand the principles of electromagnetic radiation and molecular transitions.
- Interpret selection rules using quantum and symmetry considerations.

- Analyze vibrational fine structure and electronic transitions using the Franck–Condon principle.
- Describe the principles and applications of fluorescence, phosphorescence, and circular dichroism.
- Apply advanced tools such as Mössbauer spectroscopy, and single-molecule spectroscopy.

**Course Contents (Theory):** **Credit: 2 (30 lectures)**

**Unit 1: Fundamentals & Quantum Background (6 lectures)**

Electromagnetic radiation and spectral regions. Born–Oppenheimer approximation and Uncertainty Principle. Time-dependent perturbation theory (TDPT) and transition moments. Einstein coefficients and derivation of Beer–Lambert law. Selection rules (qualitative) using symmetry and operator formalism.

**Unit 2: Electronic Spectroscopy (8 lectures)**

Electronic transitions in diatomic molecules ($\pi$–$\pi^*$, n–$\pi^*$, n–$\sigma^*$, etc.). Selection rules (qualitative). Breakdown of selection rules. Franck–Condon principle and vibrational fine structure. P, Q, R branches in rovibrational spectra. Dissociation energies (e.g. iodine spectrum).

Polyatomic molecules: Chromophores and auxochromes: structure–property relationships. Solvent effects: polarity, hydrogen bonding and solvent shifts, vibronic coupling, Charge transfer (CT) transitions and their spectral features. Qualitative interpretation of UV-Vis spectra of polyatomic organics (e.g. ethene, formaldehyde, cis- and trans-butadiene) using symmetry principles.

**Unit 3: Photophysical Processes in Molecules (6 lectures)**

Jablonski diagram, Fluorescence and phosphorescence: mechanisms and applications. Deactivation pathways, internal conversion, intersystem crossing. Mirror-image symmetry and polarization effects in emission spectroscopy.

**Unit 4: Mössbauer Spectroscopy (4 lectures)**

Mössbauer spectroscopy: Isomer shifts, quadrupole and Zeeman splitting. Applications to oxidation state and bonding.

**Unit 5: Advanced Applications (6 lectures)**

Fluorescence quenching (static/dynamic) and lifetime measurements. Single molecule spectroscopy and fluorescence correlation spectroscopy (FCS). Circular Dichroism (CD):

principle and biological examples. Mirror-image symmetry and its breakdown. Selection rules and polarization effects.

**Forward look: qualitative overview of emerging methods (e.g. AI-assisted spectra interpretation)-non-evaluative.**

**Recommended Texts/References:**


1. J. Michael Hollas, Modern Spectroscopy, 4th Ed.
2. Rita Kakkar, Atomic and Molecular Spectroscopy, Cambridge University Press
3. C. N. Banwell & E. M. McCash, Fundamentals of Molecular Spectroscopy
4. Satyanarayana, D. N., Handbook of Molecular Spectroscopy, I.K. International
5. P. Atkins & R. Friedman, Molecular Quantum Mechanics
6. Jeanne L. McHale, *Molecular Spectroscopy*
7. **J. Chem. Rev. 2021, 121, 9816–9872 –** *ML + Computational Chemistry*


**Laboratory Exercises (Practical) (atleast 10): Credits: 2**

1. Analyse UV-Vis absorption spectra of conjugated systems (e.g., β-carotene) and determine the HOMO-LUMO gap.
2. Use UV-Vis spectra of a pH-sensitive dye (e.g., phenolphthalein) to determine its $pK_a$.
3. Study the effect of structure on the UV spectra of organic compounds.
4. Study the spectra of mesityl oxide/benzophenone in different solvents and classify the observed transitions in terms of $n\rightarrow\pi^*$ and $\pi\rightarrow\pi^*$ transitions. Discuss the shift in transitions relative to those in acetone.
5. Find the stoichiometry of the charge transfer (CT) complex formed between thiocyanate ions and iron (III) by Job's method of continuous variation.
6. (a) Record the UV spectra of a weak acid (α-naphthol) at different pH and determine the dissociation constant in the ground state.

   (b) Record the fluorescence spectra of a weak acid (α-naphthol) at different pH and determine the dissociation constant in the excited state.

   Comment on the difference in the two values using MO theory.

**Instruction Mode:** Demonstration/Discussion of working principle/Hands-on with substantial literature analysis/Laboratory exercise

7. Record and compare IR spectra of alcohols in pure form and diluted in non-polar solvents to understand the effect of hydrogen bonding on O-H stretching frequency.
8. Create calibration curve and use it to determine the concentration of a fluorophore (quinine, riboflavin) in unknown samples.

9. Study UV-Vis spectra of $d^0$ transition metal complexes (e.g., $Ti^{3+}$) and assign electronic transitions using computational or experimental techniques.
10. Measure absorbance vs. time data to study the kinetics of fast photochemical reactions (using Time-Resolved Absorption Spectroscopy for Reaction Kinetics).
11. Resolve and assign vibrational fine structure in the UV-Vis spectrum of iodine vapour.
12. UV spectra comparison of substituted benzenes (π–π* vs n–π*)
13. Fluorescence quenching and lifetime (model system, Rhodamine or naphthol)
14. CD analysis of protein model (experimental or literature spectra)

15. Simulation and analysis of Franck–Condon transitions using potential energy diagrams for diatomic molecules.

16. Interpret Mössbauer isomer shift and quadrupole splitting data from literature spectra of iron complexes.

**Recommended Texts/References:**


1. Rita Kakkar, Atomic and Molecular Spectroscopy, Cambridge University Press.
2. B. D. Khosla, V. C. Garg, A. Gulati, Senior Practical Physical Chemistry, R. Chand & Co., New Delhi.
3. Donald A. McQuarrie & John D. Simon, Physical Chemistry: A Molecular Approach.
4. J. Michael Hollas, Modern Spectroscopy.
5. Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis.
6. Jeanne L. McHale, Molecular Spectroscopy.

**<u>DISCIPLINE SPECIFIC ELECTIVE COURSE-II (DSE-II):</u>**

**<u>Title</u>: Interfaces, Macromolecules and Biophysical Chemistry (DSE-II, Semester-VII, 30 Lectures)**

| Course title & Code | Credits | Credit distribution of the Course | | | Eligibility criteria | Pre-requisite of the course (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Interfaces, Macromolecules and Biophysical Chemistry (DSE-II, Semester-VII, 30 Lectures) | 04 | 02 | --- | 02 | Class 12th with Physics, Chemistry, Mathematics | --- |

**<u>Course Objectives:</u>**

- To understand fundamental surface and interfacial phenomena including adsorption, wetting, and catalysis.
- To introduce classification and characterization of polymers, polymerization mechanisms, and molecular weight determination.
- To apply thermodynamics and kinetics to protein folding, ligand binding, and enzyme catalysis.
- To familiarize students with analytical and optical tools used to study biomolecular structure and interactions.
- To bridge molecular understanding with biological function through biophysical chemistry.

**<u>Learning outcomes</u>:** By the end of the course, students will be able to:

- Explain micellization, surface tension, adsorption isotherms, and thin film properties.
- Describe polymer synthesis, types, and methods for determining molecular weights.
- Analyze biological macromolecules using thermodynamic, kinetic, and statistical models.
- Use key spectroscopic and separation techniques to investigate biomolecular properties.
- Connect experimental methods with structural and functional insights in biophysical chemistry.

**Course Contents (Theory):** **Credit: 2 (30 lectures)**

**Unit-I: Surface and Interface Chemistry (8 lectures)**

Surface-active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Krafft temperature.
Packing parameters, thermodynamics of micellization, solubilization, reverse micelles. Electrokinetic phenomena, Young-Laplace and Kelvin equations.
Adsorption: - Gibbs adsorption isotherm, Langmuir and BET isotherms, surface area measurements.
Thin films and Langmuir-Blodgett films.
Catalytic activity at surfaces (overview).

**Unit II: Polymer Structure and Characterization (8 lectures)**

Macromolecules and types of polymerizations, Degree of polymerization, number and mass average molecular masses, Polymer characterization: osmometry, viscometry, light scattering, diffusion.
Glass transition temperature, crystallinity.

**Unit III: Biophysical Chemistry of Macromolecules (8 lectures)**

Isoelectric point of amino acids, Configuration, and conformation of biological macromolecules, Thermodynamics of protein folding/stability, Configurational statistics and conformational transitions, Thermodynamics and kinetics of ligand interactions, Macromolecule-ligand binding and cooperativity (including Hill equation).

Enzyme catalysis: Michaelis-Menten equation (with derivation), Lineweaver-Burk plot, define the turnover number and Michaelis constant, Enzyme inhibition- reversibility and products inhibition

**Unit IV: Spectroscopic and Analytical techniques(3 lectures)**

Basic principles and applications of analytical and optical techniques in biological systems: Absorption and fluorescence spectroscopy (overview only), Isothermal Titration Calorimetry

(ITC), Linear and Circular Dichroism (CD), Single and multidimensional NMR spectroscopy. Single molecule spectroscopy.

**Unit V: Separation techniques (3 lectures)**

Methods for the separation of biomolecules: General principles, including Chromatography; Sedimentation, Moving Boundary Sedimentation, Zonal Sedimentation, Electrophoresis, Isoelectric focusing, Capillary electrophoresis, MALDI-TOF.

**Recommended Texts/References:**


1. Adamson, A. W. & Gast, A. P., Physical Chemistry of Surfaces, 6th Ed., Wiley
2. Somorjai, G. A. & Li, Y., Surface Chemistry and Catalysis
3. Israelachvili, J. N., Intermolecular and Surface Forces
4. Carraher, C. E., Introduction to Polymer Chemistry
5. Odian, G., Principles of Polymerization
6. Cantor, C. R. & Schimmel, P. R., Biophysical Chemistry (3 vols)
7. Wilson, K. & Walker, J., Principles and Techniques of Biochemistry and Molecular Biology
8. Dill, K. A. & Bromberg, S., Molecular Driving Forces
9. Hiemenz, P. C. & Lodge, T. P., Polymer Chemistry
10. Hiemenz, P. C. & Rajagopalan, R., Principles of Colloid and Surface Chemistry
11. Van Holde, Principles of Physical Biochemistry


**Laboratory Exercises (Practical) (atleast 10):** **Credit: 2**

1. Study of adsorption of Acetic Acid on Charcoal.
2. Conductometric Study of Critical Micellar Concentration.
3. Calculation of the thermodynamic parameters of micellization of SDS surfactant from conductivity/spectroscopic measurements.
4. Determination of $pK_a$ values and the isoelectric point of an amino acid (both acidic and basic) using pH titration against acid and base.
5. Determination of surface area of a surfactant molecule using Gibbs adsorption isotherm.
6. Study of the catalytic efficiency of a non-specific enzyme by measuring the rate of the enzyme-catalysed reaction.
7. Separation of serum proteins using paper electrophoresis/ Ammonium Sulphate fractionation.
8. Molecular docking study for binding interaction of Fluconazole with 14a-demethylase enzyme (lanosterol) of prominent fungal pathogens Candida albicans using protein structure from protein data bank (PDB ID: CYP51) and Open-source software i.e. AutoDock Vina/ Swiss Dock, etc.

**Instruction Mode:** Demonstration/ Discussion of working principle/ Hands-on with substantial literature analysis/ Laboratory exercise

9. Instruction mode transaction of working principle of CD spectroscopy and demonstrating experimental protocol for determining protein folding and the percent helix, sheet, turns, and random structure change in protein (Bovine Serum Albumin) upon binding with a suitable ligand i.e. Rhodamine B.
10. Instruction mode transaction of working principle of MALDI-TOF instrumentation technique and its application to identify serum proteins (i.e. Bovine Serum Albumin) and their post translational modifications.
11. Instruction mode transaction of working principle of fluorescence spectroscopy and demonstrating experimental protocol for designing fluorescence/phosphorescence-based chemo sensors for detection of amino acid arginine.
12. Experimental Demonstration of the thermodynamics of urea induced denaturation of a protein, bovine serum albumin, by using fluorimetry.

**Recommended Texts/References:**


1. Voet, D.; Voet, J. G.; Pratt, C. W. Fundamentals of Biochemistry (Fifth Edition), John Wiley & Sons, Inc.
2. Lakowicz, J. R.; Principles of Fluorescence Spectroscopy, Springer Nature; 3rd edition (4 August 2006).
3. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
4. Hiemenz, P. C.; Rajagopalan, R. Principles of Colloid and Surface Chemistry (3rd Edition) MarceldEkkerin, C.
5. Adamson, A. W.; Gast, A. P.; Physical Chemistry of Surfaces, Sixth Editions, John Wiley & Sons, Inc.

**DISCIPINE SPECIFIC ELECTIVES-IV (DSE-III)**

**Title: Mathematical Methods in Chemistry (DSE -III, Semester-VII, 30 Lectures)**

| Course title & Code | Credits | Credit distribution of the Course | | | Eligibility criteria | Pre-requisite of the course (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Mathematical Methods in Chemistry (DSE -III, Semester-VII, 30 Lectures) | 04 | 02 | --- | 02 | Class 12th with Physics, Chemistry, Mathematics | --- |

**Course Objectives:**

- To build a working knowledge of essential mathematical tools used in physical chemistry.
- To develop confidence in applying calculus, algebra, and probability in thermodynamics, kinetics, and spectroscopy.
- To illustrate concepts with examples relevant to chemical phenomena.

**Learning outcomes:** After completing the course, the student will be able to:

- Use vector and matrix operations to solve chemical problems (e.g., molecular orbitals, symmetry).
- Understand and apply vector calculus to thermodynamic and electrostatic systems.
- Solve differential and integral problems relevant to kinetics and quantum chemistry.
- Apply probability and curve-fitting concepts to experimental data analysis.
- Understand the role of eigenvalues and coordinate transformations in physical chemistry models.

**Course Contents (Theory):** **Credit: 2 (30 Lectures)**

**Unit I: Vectors and Matrix Algebra (10 lectures)**

Vectors: Dot, cross, and triple products

Vector calculus: Gradient, divergence,and curl.

Integral theorems: Gauss' and Stokes' theorem (physical interpretation only).

Matrices:Types (square, diagonal, identity), operations (addition, multiplication, transpose), Inverse and adjoint.

Special matrices: Symmetric, skew–symmetric, Hermitian, skew- Hermitian, unitary-properties and physical relevance (e.g., Hermitian in quantum mechanics).

Determinants: Evaluation (2x2, 3x3 only), properties, Cramer's rule.

Eigenvalues and eigenvectors: Definition and physical meaning, Diagonalization with examples from Hückel theory and moment of inertia tensor.

Second-rank tensors (conceptual only): Brief mention of how second-rank tensors like polarizability and magnetic susceptibility help describe molecular properties.

**Unit II: Differential and Integral Calculus (8 lectures)**

Functions, continuity and differentiability, rules for differentiation. Exact and inexact differentials with their applications to thermodynamic properties.

Differentiation and chemical applications, including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution, etc).

Partial differentiation, coordinate transformations (for example,cartesian to spherical polar).

Basic rules for integration, integration by parts, substitution, partial fractions and substitution, reduction formulae. Applications of integral calculus.

Curve sketching and thermodynamic functions.

**Unit III: Differential Equations (7 lectures)**

First order differential equations: separable, linear, exact.

Applications to rate laws and chemical equilibrium.

Second-order differential equations: harmonic oscillator, Legendre equation (qualitative)

Introduction to Fourier series and boundary value problems (qualitative).

Examples from quantum chemistry (H-atom, angular momentum)

**Unit IV: Probability, Statistics, and Curve Fitting (5 lectures)**

Permutations and combinations

Probability distributions, RMS, mean, most probable values (Maxwell-Boltzmann distribution).

Error analysis in chemical experiments (standard deviation, RMS error)

Least squares fitting, polynomial trendlines (chemical data)

**Recommended Texts/References:**

1. Martin C. R. Cockett and Graham Doggett, Math for Chemist: Volume 1&2, Royal Society of Chemistry, Thomas Graham House, Cambridge, UK, 2003.
2. Robert G. Mortimer, Mathematics for Physical Chemistry, Elsevier

**Supplementary Reading**

1. McQuarrie, D. A., Mathematical methods for scientists and engineers, University Science Books, 2003.
2. Arfken, G., Weber, H., and Harris, F., Mathematical methods for physicists, Academic Press, 7th Ed., 2012.
3. Boas, M. L., Mathematical methods for the physical sciences, Kaye Pace, 3rd Ed., 2006.

**Laboratory Exercises (Practical)/Tutorials:** **Credit: 2**

1. Least-squares fit: Linear regression for absorbance vs. concentration data.
2. Matrix multiplication: Three-matrix multiplication, Group theory example.
3. Diagonalization: Secular determinant from Hückel Theory
4. Error analysis: Calculate SD, RMS error, correlation from experimental data.
5. Differential calculus: Maxima/minima problems (e.g., Boltzmann populations).
6. Integral calculus: Evaluation of thermodynamic integrals (e.g., partition functions).
7. Differential Solve and interpret rate equations, harmonic oscillator.
8. Curve fitting: Polynomial fit using spreadsheet or Python (optional).

**Recommended Texts/References:**

1. Cockett & Doggett, *Maths for Chemists*, Vols 1 & 2 (Royal Society of Chemistry)
2. Robert G. Mortimer, *Mathematics for Physical Chemistry*
3. McQuarrie & Simon, *Physical Chemistry: A Molecular Approach* (selected examples)
4. Excel or Google Sheets for plotting; Python (optional)

## SEMESTER – VIII

## DISCIPLINESPECIFICELECTIVECOURSE-3(DSE-3):

## Transition Metal Clusters-Introduction and Applications

### CREDITDISTRIBUTION,ELIGIBILITYANDPRE-REQUISITESOFTHE COURSE

| Coursetitle & Code | Credits | Creditdistributionofthe course | | | Eligibility criteria | Pre-requisite ofthecourse (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical / Practice | | |
| **Transition Metal Clusters-Introduction and Applications (DSE-3)** | **04** | **02** | **--** | **02** | Class12th with Physics, Chemistry, Mathematics, | **--** |

**Objectives:**

To introduce the basic concepts of transition metal clusters. To gather a good understanding of the chemistry and various aspects of metal-carbonyl clusters, carboranes, metalloboranes and heteroboranes, metallocarboranes with respect to synthesis, structure and properties.

**Learning Outcomes:**

On completion of the course, the students will be able to:

- Ensures the students understand the concepts and the properties of transition metal clusters.
- Acquire knowledge of transition metal clusters cluster compounds and explain structure-property, electron counts, and surface analogies of cluster compounds.
- Identify the structure and bonding aspects of transition metal clusters.
- Identify the different types of transition metal clusters reactions and apply the above concepts to explain reactivity of the clusters.
- To study the application of molecular clusters in catalysis.

### SYLLABUSOFDSE-3

Transition-metal clusters: Low nuclearity metal-carbonyl clusters and 14n+2 rule, high nuclearity metal-carbonyl clusters with internal atoms, polyhedral skeletal electron pair theory

(PSEPT), metalloboranes, metallocarboranes. Structure, synthesis, bonding aspects and reactivity. Capping rules, metal-ligand complexes vs heteronuclear cluster.

Main-group-Transition-metal clusters: Isolobalanalogs of p-block and d-block clusters, limitations and exceptions.

Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters. Chevrel compounds, infinite metal chains, multidecker molecules-cluster surface analogy.

Molecular clusters in catalysis, clusters to materials.Illustrative examples from recent literature.(30 Lectures)

**Keywords:** Transition Metal Clusters, metal-carbonyl clusters, carboranes, metalloboranes, heteroboranes, metallocarboranes, Capping rules, Isolobal relationship, interstitial main group elements, cubane clusters and naked or Zintl clusters, Chevrel compounds, catalysis, clusters to materials, boron-carbides, metal-borides, Synthesis, Reactivity.

**Teaching Learning Process:**

Lectures, ICT enabled teaching, presentations by students, group discussion and quiz will be the part of teaching learning process.

**Assessment Methods:**

● Presentations by Individual Student/ Group of Students

● Class Tests at Periodic Intervals.

● Written assignment(s)

● End semester University Theory Examination

**Practicals**

1. Synthesis of ferrocene and its characterisation using IR, $^1$H NMR and UV-Visible spectroscopy
2. Synthesis of acetylferrocene and its characterisation using IR, $^1$H NMR and UV-Visible spectroscopy
3. Synthesis of $[Fe(\eta\text{-}C_5H_5)(\eta\text{-}C_6H_6)]PF_6$ using ligand exchange reaction. Characterisation of the product using IR, $^1$H NMR and UV-Visible spectrum
4. Estimation of metal ions in the mixture solution- $Mg^{2+}$- $Zn^{2+}$, $Ca^{2+}$- $Mg^{2+}$, $Cu^{2+}$ - $Zn^{2+}$titrimetrically.
5. Analysis of given transition metal cluster(metal carbonyls) using various spectroscopic techniques - IR, UV-Visible and mass spectrometry.

**Text Books:**


1. M. P. Mingos and D. J. Wales; Introduction to Cluster Chemistry, Prentice Hall, 1990.

2. N. Greenwood and E. A. Earnshaw; Chemistry of elements, Second Edition, Butterworth-Heinemann, 1997.
3. P. Fehlner, J. F. Halet and J-Y. Saillard; Molecular Clusters: A Bridge to solid-state Chemistry, Cambridge University press, 2007.
4. D. Gupta and A. J. Elias; Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, Universities Press (India), 2010.
5. M. P. Mingos, Essential Trends in Inorganic Chemistry, Oxford, University Press, 1998.
6. C.E. Housecroft, Metal-Metal Bonded Carbonyl Dimers and Clusters, Oxford Chemistry Primers (44), Oxford, University Press, 1996.

**Reference Books:**

1. F. Holleman and E. Wifrg, Inorganic Chemistry, Academic Press, New York, 1995.
2. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn, John Wiley & Sons, Inc, New York, 1999.
3. G. Wulfsberg, Inorganic Chemistry, Viva Books Pvt Ltd, New Delhi, 2001.
4. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.
5. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Shriver & Atkins Inorganic Chemistry, 4th Edn, Oxford, 2006.
6. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Inorgnic Chemistry: Principles of Structures and Reactivity, 4th Edn, Pearson, New Delhi, 2006.
7. R. Xu, W. Pang and Q. Huo (Eds), Modern Inorganic Synthetic Chemistry, Elsevier, New York, 2011.
8. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd Edn, Pearson, New Delhi, 2009.
9. J. R. Anderson and M. Boudart (Eds), Catalysis: Science and Technology, Springer, London, 2012.
10. P. Powell, Principles of Organometallic Chemistry, 2nd Edn, Chapman and Hall, London, 1988.
11. G. O. Spessard and G. L. Miessler, Organometallic Chemistry, International 2nd Edn, Oxford University Press, Oxford, 2010.
12. D. F. Shriver, H. D. Kaesz and R. D. Adams (Eds), The Chemistry of Metal Cluster Complexes, VCH, New York, 1990.
13. K. J. Klabunde, Free Atoms, Clusters and Nanoscale Particles, Academic Press, New York, 1994.
14. D. M. P. Mingos (Ed.), Structural and Electronic Paradigms in Cluster Chemistry, Springer, Berlin, 1997.
15. P. Braunstein, L. A. Oro and P. R. Raithby (Eds), Metal Clusters in Chemistry, Wiley-VCH, Weinheim, 1999.
16. M. Driess and H. Noth (Eds), Molecular Clusters of the Main Group Elements, Wiley-VCH, Weinheim, 2004.

17. C. E. Housecraft and A. G. Sharpe, Inorganic Chemistry, 3rd Edn, Pearson Education Ltd, Essex, England, 2008.
18. F. Wells, Structural Inorganic Chemistry, 5th Edn, Oxford University Press, Oxford, 1984.

## DISCIPLINESPECIFICELECTIVECOURSE-4(DSE-4):

## Advanced Analytical Techniques for Inorganic Compounds

### CREDITDISTRIBUTION,ELIGIBILITYANDPRE-REQUISITESOFTHE COURSE

| Coursetitle & Code | Credits | Creditdistributionofthe course | | | Eligibility criteria | Pre-requisite ofthecourse (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical /Practice | | |
| **Advanced Analytical Techniques for Inorganic Compounds (DSE-4)** | **04** | **02** | **--** | **02** | Class12th with Physics, Chemistry, Mathematics, | **--** |

**Learning Objectives**

This course is to equip students in handling advanced analytical instruments and techniques important for analysing inorganic compounds.

**Learning outcomes**

- By the end of the course, the students will be able to:
- To apply the fundamentals of various types of spectroscopic techniques like UV, IR, EPR and Mossbauer spectroscopy and applications of these techniques to interpret data.
- To describe the advancement in spectroscopic methods like IR, UV, EPR and Mossbauer and can recognize necessity of these techniques in the field of analytical science.
- To perform quantitative and qualitative measurements of samples by IR, UV.
- To use different techniques like liquid-liquid extraction, counter current extraction, digestion and solid phase extraction for sample preparation
- To be able to identify, recognize and compare principle, instrumentations and application of Atomic Absorption Spectroscopy (AAS), inductively coupled plasma atomic emission spectroscopy (ICP-AES),

### SYLLABUSOFDSE-4

**Unit 01**- Purification and drying of solvent. Reagents used in undergraduate laboratory: preparation, purification and handling. (04 Lectures)

**Unit 02** – Introduction, Physical and Chemical Principles, Spectrometers, Detection, Calculation, and Output, Analytical Information: Qualitative and Quantitative, Applications

Instrumental techniques in laboratory: Infrared spectrophotometer, UV-Visible spectrophotometer. Column chromatography and metal ions separation through ion exchange chromatography.(10 Lectures)

**Unit 03**- Atomic Absorption and Emission Spectrometry

Introduction, hollow cathode lamp as a source and its working, premix chamber burner and total consumption burner, Flame atomizer - principle and working mechanism of electrothermal atomizers, line width, different interferences observed in AAS. Inductively Coupled Plasma Atomic Emission Spectroscopy.(10 Lectures)

**Unit 04**: Introduction to EPR and Mossbauer spectroscopy andtheir Applications

(06 Lectures)

**Keywords:**Solvent, Reagents Infrared spectrophotometer, UV-Visible spectrophotometer. Column chromatography, Ion exchange chromatography, AAS, ICP-AES, EPR and Mossbauer spectroscopy

**Teaching Learning Process:**

Lectures, ICT enabled teaching, presentations by students, group discussion and quiz will be the part of teaching learning process.

**Assessment Methods:**

- Presentations by Individual Student/ Group of Students
- Class Tests at Periodic Intervals.
- Written assignment(s)
- End semester University Theory Examination

**Practical:**

1. Preparation of VO (acac)$_2$ and its characterisation by determining magnetic moment, UV-Visible and IR spectroscopy.
2. Separation of $Ni^{2+}$ and $Zn^{2+}$ in the given mixture through column chromatography.
3. Preparation of $[Co(en)_3]Cl_3$ , *cis*- and *trans*- $[Co(en)_2Cl_2]Cl$by oxidation of $Co^{2+}$and measurement of their optical activity.
4. Spectrophotometric estimation of $Cr^{3+}$ in the given solution by 1,5-diphenylcarbazide
5. Estimation of $Cu^{2+}$-$Fe^{3+}$/$Cu^{2+}$-$Bi^{3+}$ in the mixture solution with EDTA spectrophotometrically.
6. Synthesis of any ligand of choice (for example- carboxylate, ester, Schiff base, amides, amines etc.).

7. Synthesis of a transition metal complex using above ligand
8. Characterisation of above complex using suitable analytical technique
9. To determine the solubility and solubility product of a sparingly soluble electrolyte conductometrically.

**References for both theory and practical**


1. Fundamentals of Analytical Chemistry by Crouch, West and Skoog,9th edition , Brooks/Cole(2013)
2. Analytical Chemistry, Gary D. Christian, 6th Edition, John Wiley and Sons Inc. New Jersey,2007.
3. Instrumental Methods of Chemical Analysis, by Galen W. Ewing, 4thEdition, International Student Edition, 1969.
4. Instrumental methods of analysis, 7th Ed, Willard, Merritt, Dean, SettleCBS Publishers & Distributors 2004.
5. Advanced practical inorganic chemistry, D.M. Adams, J.B. Raynor John Wiley & Sons Ltd 1965
6. Advanced practical organic chemistry, 2nd Ed. Leonard, Lygo, Procter.CRC Press; 3rd edition 2013
7. Inorganic experiments, J.D. Woollins, Wiley VCH 2009
8. General Chemistry Experiments. Anil J. Elias, universities press,2016.
9. Fundamentals of Analytical Chemistry, Skoog and West's, 9th Edition, Cengage Learning Publisher, 2014.
10. Analytical Chemistry-An Indian Adaption,Gary D Christian, Purnendu K Dasgupta, Kevin A Schug , Wiley India Pvt.Ltd,2020.
11. Specrochemical Analysis by Atomic Absorption and Emission, Lajunen L H J, Cambridge, UK: The Royal Society of Chemistry, 1992.
12. Advances in Atomic Spectroscopy, Sneddon J, CT: JAI Press, Greenwich, 1992.
13. CRC Handbook of Inductively Coupled Plasma Atomic Emission Spectrometry, Varma A, FL: CRC Press, Boca Raton, 1991.


# GE (2+2) Credit

# The existing pool of GE papers of Chemistry can be extended to VII and VIII semesters.

# DISCIPLINE-SPECIFIC ELECTIVE COURSE-III (DSE-III)

## Title: Fundamentals of Natural Products (DSE-III, Semester-VIII, 30 Lectures)

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

| Coursetitle &Code | Credits | Credit distribution of theCourse | | | Eligibility criteria | Pre-requisite (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Fundamentals of Natural Products (DSE-III, 30 Lectures) | 04 | 02 | --- | 02 | Class 12$^{th}$with Physics,Chemistry, Mathematics | |

***Objectives:***The primary objective of this course is to provide students with a comprehensive understanding of natural product chemistry, including its historical development, modern applications, classification, biosynthesis, and methods for isolation and purification.

***Outcomes:***By the end of this course, students will understand the scope and significance of natural product chemistry in both historical and modern contexts, particularly its role in drug discovery. Students will classify major natural product groups-such as alkaloids, terpenoids, flavonoids, phenolics, peptides, glycosides, polyketides, steroids, and hormones-and understand their structures and functions.

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***Theory Course Content*** ***2 Credit (30 lectures)***

***Introduction***:Definition and scope of natural product chemistry, historical significance and modern relevance, Primary vs secondary metabolites, Sources of natural products: terrestrial and marine origin, importance in drug discovery and development.**(4 Lectures)**

***Classification of Natural Products***:Alkaloids, Terpenoids, Flavonoids, Phenolics, Peptides and Proteins, Glycosides, Polyketides, Steroids and Hormones (structure and function only).Isoprene rule, mevalonate and non-mevalonate pathways, Shikimic acid pathway. **(7 Lectures)**

***Isolation and Purification Techniques***:Extraction methods (solvent extraction, Soxhlet, maceration, etc.), Chromatographic techniques (TLC, Column, HPLC, GC-MS), Crystallization and distillation techniques, Bioassay-guided fractionation.**(4 Lectures)**

***Total Synthesis of Natural Products:*** Artemisinin (Antimalarial);Berberine (anti-inflammatory); Lysergic Acid Diethylamide(Psychedelic drug). **(10 Lectures)**

***Biosynthesis of Natural Products***:Artemisinin, Berberine, and Lysergic Acid Diethylamide (LSD). **(5 Lectures)**

***Recommended Reference and Textbooks:***

1. Mann, J.; Davidson, R. S. & Hobbs, J. B.,**Natural Products: Their Chemistry and Biological Significance, Longman Scientific & Technical (1994)**
2. Mann, J. Secondary Metabolites, Oxford University Press, Oxford, UK, (**1980**)
3. Hanson, J. R., **Natural Products:The Secondary Metabolites, The Royal Society of Chemistry, Cambridge, UK (2003)**
4. Chatwal, G.,**Organic Chemistry of Natural Products, Himalaya Publishing House (1994)**

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## PRACTICALS

***Course Outcome*:** The students will acquire knowledge of:

**1.** To isolate natural alkaloids using solvent extraction.
**2.** Characterization by physical and spectroscopic techniques.

| ***List of Practical's*** | ***2 Credit*** |
|---|---|

**1.** Isolation of natural products: Isolation of $\beta$-carotene from carrots.
**2.** Isolation of natural products: Isolation of caffeine from tea leaves.
**3.** Isolation of natural products: Isolation of piperene from black pepper.
**4.** Isolation of natural products: Isolation of eugenol from cloves.
**5.** Synthesis of 7-hydroxy-4-methylcoumarin
**6.** Synthesis of a simple dipeptide(gly-gly)by DCC coupling using N-protected amino acids.
**7.** Synthesis of simple amino acids

***Recommended Reference and Textbooks:***

**1.** Vogel, A. I. (**2012**), Quantitative Organic Analysis, Part 3, Pearson Education.
**2.** Mann, F. G., Saunders, B.C. (**2009**), Practical Organic Chemistry, Pearson Education.
**3.** Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (**2012**), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
**4.** Ahluwalia, V.K., Dhingra, S. (**2004**), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
**5.** Ahluwalia, V. K., Aggarwal, R. (**2004**), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
**6.** Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
**7.** Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi

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# DISCIPLINE-SPECIFIC ELECTIVE COURSE-IV (DSE-IV)

## Title: Fundamentals of Medicinal Chemistry (DSE-IV, 30 Lectures)

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

| Coursetitle &Code | Credits | Credit distribution | | | Eligibility criteria | Pre-requisite (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Fundamentals of Medicinal Chemistry (DSE-III, 30 Lectures) | 04 | 02 | --- | 02 | Class 12$^{th}$with Physics,Chemistry, Mathematics | |

***Objectives:*** This course aims to introduce students to the foundational concepts of medicinal chemistry, highlighting its historical development and the significance of natural products as drug sources. Additionally, the course examines the structure, synthesis, therapeutic use, and basic SAR of key drugs like Ibuprofen, Paracetamol, Aspirin, and Penicillin.

***Outcome:*** By the end of the course, students will be able to explain the development and role of medicinal chemistry, understand the stages of drug discovery, and evaluate drug screening and clinical processes. They will interpret how stereochemical and physicochemical properties influence drug behavior and efficacy.

***Theory Course Content*** ***2 Credit (30 Lectures)***

***Introduction****:* History and development of medicinal Chemistry. Sources of drugs, including natural products with examples, Stages of drug discovery, Stereochemical aspects, Physicochemical properties: solubility, acid-base, partition coefficient. (**7 Lectures**)

***Drug discovery***: Target identification and validation, Screening of drugs, High throughput screening (HTS), Random and Systematic screening. Structure activity relationship (SAR), Hit identification, and Lead optimization. ` (**8 Lectures**)

***Pharmacokinetics (ADME)****:* Drug administration/absorption, drug distribution, drug metabolism - Phase 1 and Phase 2, drug excretion, Half-Life of drugs, and Clinical trials. (**5 Lectures**)

***Representative Synthetic Drugs****:*Structure, Synthesis, and Therapeutic Valueof Representative Drugs:Fluconazole (antifungal), Penicillin (antibiotic), Isoniazid (antibiotic),and Azidothymidine (AZT; anti-HIV). (**7 Lectures**)

***Bioinformatics****:*Use of computational tools for drug design.(**3 Lectures**)

***Recommended Texts:***

**1.** Patrick, G. L. *Introduction to Medicinal Chemistry*, Oxford University Press (2001)

2. Lemke, T. L. & William, *D. A., Foye's Principles of Medicinal Chemistry*, 5th Ed., USA (2002)
3. Dunlap, N. K. &Huryn, D. M., *Medicinal Chemistry*, Garland Science, New York (2018)
4. Mark W. Holladay, Richard B. Silverman.*The Organic Chemistry of Drug Design and Drug Action,* 3rd Ed. Academic Press (**2014**)

# PRACTICALS

***Course Outcome:*** The students will acquire knowledge of:

1. Synthesis and isolation of active ingredients and biologically active compounds/drugs.
2. Characterizationof active ingredients by physical and spectroscopic techniques.
3. Basic drug designing using computational methods

| ***List of Practical's*** | ***2 Credit*** |
|---|---|

1. Isolation and estimation of aspirin from commercial tablets
2. Synthesis of paracetamol from *p*-aminophenol
3. Synthesis of benzotriazole/benzimidazole.
4. Synthesis of 5,5'-Diphenylhydantoin.
5. Synthesis of dihydropyridine (DHP)/dihydropyrimidine (DHPM).
6. Study of physicochemical properties of pharmaceutically active compounds using computational methods.

***Recommended Reference and Textbooks:***

1. Vogel, A. I. (**2012**), Quantitative Organic Analysis, Part 3, Pearson Education.
2. Mann, F. G., Saunders, B.C. (**2009**), Practical Organic Chemistry, Pearson Education.
3. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (**2012**), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
4. Ahluwalia, V. K., Dhingra, S. (**2004**), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
5. Ahluwalia, V. K., Aggarwal, R. (**2004**), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
6. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
7. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi

**DISCIPLINE SPECIFIC ELECTIVE COURSE-IV (DSE-IV):**

**Title: Interfacial Electrochemistry (DSE-IV, Semester-VIII, 30 Lectures)**

| **Course title & Code** | **Credits** | **Credit distribution of the course** | | | **Eligibility criteria** | **Pre-requisite of the course (if any)** |
|---|---|---|---|---|---|---|
| | | **Lecture** | **Tutorial** | **Practical/ Practice** | | |
| **Interfacial Electrochemistry (DSE-IV, Semester-VIII, 30 Lectures)** | **04** | **02** | **---** | **02** | **Class 12th with Physics, Chemistry, Mathematics** | **---** |

**Course Objectives:**

- To introduce the structure and thermodynamics of electrochemical interfaces including models of the electric double layer.
- To explain electrode kinetics with emphasis on Butler-Volmer kinetics, Tafel plots, and cyclic voltammetry.
- To introduce Marcus theory and concepts of electrocatalysis and corrosion with real-world relevance.
- To explain transport in electrolyte solutions using laws of diffusion laws, Debye-Hückel theory, and transport numbers.
- To explore adsorption thermodynamics and applications of electrochemical principles in energy storage and conversion devices.

**Learning Outcomes:**

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

- Explain and compare models of electric double layer and relate them to interfacial properties.

- Apply the Butler-Volmer equation and cyclic voltammetry to interpret reaction mechanisms.
- Describe Marcus theory and the role of parameters in HER, OER and corrosion control.
- Interpret adsorption isotherms and thermodynamic data related to interface processes.
- Evaluate electrochemical energy devices like fuel cells, batteries and supercapacitors.

**Course Contents (Theory):** **Credit: 2 (30 lectures)**

**Unit I: Structure and Thermodynamics of Electrochemical Interface (5 lectures)**

Overview of interfaces and electrochemical systems.Electric Double Layer: Models: Helmholtz Model, Gouy-Chapman Model (derivation), Stern Model, Graham-Devanathan-Mott-Watts model, Tobin, Bockris-Devanathan model, Thermodynamics of the EDL

Electrocapillary phenomena

**Unit II: Electrode Kinetics and Cyclic Voltammetry (6 lectures)**

Standard, formal and equilibrium potentials, Overpotentials and their types, Butler-Volmer equation: Derivation and its physical implications, Exchange current density and transfer coefficient, Tafel equation and graphical interpretation, Cyclic voltammetry: Theory and experimental design. Distinguishing reversible, quasi-reversible, irreversible, and capacitive processes.

**Unit III: Electron Transfer and Electrocatalysis (4 lectures)**

Marcus theory (qualitative description only): activationless region, reorganization energy

Introduction to electrocatalysis, Parameters influencing HER, OER, and oxygen reduction reaction (ORR), Role of electrode materials.

**Unit IV: Transport in Electrolytes (5 lectures)**

Ionic mobility and transport number, Fick's laws of diffusion, Einstein equation for diffusion

Debye–Hückel–Onsager limiting law, Electrophoretic and relaxation effects, time of relaxation

Dependence of transport number on concentration

**Unit V: Adsorption and Surface Thermodynamics (3 lectures)**

Adsorption of ions and molecules at interfaces, Thermodynamic treatment of adsorption

Adsorption isotherms:Langmuir, Frumkin, Temkin, Determination of surface excess and charge

**Unit VI: Corrosion and its Control (3 lectures)**

Types of corrosion: uniform, galvanic, pitting, crevice, etc., Thermodynamics and kinetic aspects.Monitoring methods: electrochemical noise, impedance, Inhibition and protective coatings.

**Unit VII: Electrochemical Energy Conversion and Storage (4 lectures)**

Fuel cells: PEMFC, Alkaline, Methanol, Batteries: Lithium-ion, Redox flow

Supercapacitors: EDLC and pseudocapacitors. Comparative performance and limitations

**Recommended Texts/References:**


1. Bard, A. J. Faulkner, L. R. Electrochemical Methods: Fundamentals and Applications, 2nd Ed., John Wiley & Sons: New York, 2002.
2. Oldham, K. B., Myland, J. C. and Bond, A. M. Electrochemical Science and Technology: Fundamental and Applications, John Wiley & Sons, Ltd. (2012).
3. Bagotsky, V.S., Fundamentals of electrochemistry 2nd Ed. Wiley – Interscience, (2006)


**Supplementary References**


1. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 1: Ionics 2nd Ed., Springer (1998).
2. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science 2nd Ed., Springer (2001).
3. Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E. Modern Electrochemistry 2A: Fundamentals of Electrodics 2nd Ed., Springer (2001).
4. Brett, C. M. A. & Brett, A. M. O. Electrochemistry, Oxford University Press (1993).
5. Koryta, J., Dvorak, J. & Kavan, L. Principles of Electrochemistry John Wiley & Sons: NY (1993).
6. Hamann, Carl H., Hamneff, Andrew &Vielstich, Wolf., Electrochemistry, 2nd Ed. (2007)


**Laboratory Exercises (Practical) (atleast 10:** **Credit: 2**

1. Conductometric Titration of a Charge Transfer System, the formation of charge transfer complex between an electron donor and acceptor is studied and the stoichiometry of the complex is determined by following the variation of conductance of the solution with concentration of the donor and acceptor.
2. Study of the oscillating reaction using the $Ce^{3+}/Ce^{4+}$ system; and the dependence of the oscillation period on the metal ion concentration.
3. Intercalation of sodium into vanadium oxide and potentiometric estimation of extent of intercalation.
4. Effect of ionic strength on reaction rate (persulfate-iodine reaction).
5. Potentiometric determination of solubility and solubility product of AgCl(s) in water.

6. Potentiometric determination of mean ionic activity coefficient of HCl at different concentrations.
7. Potentiometric titration of Phosphoric acid vs NaOH.
8. Determination of dissociation constant of acetic acid from its potentiometric titration curve.

**Instruction Mode:**Demonstration/ Discussion of working principle/ Hands-on with substantial literature analysis/ Laboratory exercise

9. Record cyclic voltammogram for the electrochemical capacitors (electric double layer) response with varying scan rates,

i) plot anodic and cathodic plateau currents vs scan rates.

(Use aqueous solution of 1.5 M $NaNO_3$)

10. Record cyclic voltammogram for a reversible heterogeneous electron transfer system with varying scan rates,

(i) Determine anodic and cathodic peak current ratio.

(ii) Determine anodic and cathodic peak potential difference.

(iii) Plot peak current vs square root of scan rates.

(Use aqueous solution of 10 mM $K_4Fe(CN)_6$ + $K_3Fe(CN)_6$ + 1.5 M $NaNO_3$ )

11. Record cyclic voltammogram for a quasi-reversible heterogeneous electron transfer system with varying scan rates,

(i) Determine anodic and cathodic peak current ratio.

(ii) Determine anodic and cathodic peak potential difference.

(iii) Plot peak current vs square root of scan rates.

(Use aqueous solution of 10mM $Fe(NH_4)_2$ $(SO_4)_2$ + $Fe(NH_4)(SO_4)_2$ + 1 M $HClO_4$)

12. Record the CV of aqueous solution of sulphuric acid (0.5 M) at Pt electrode as working electrode and counter electrode.

(i) Interpret and explain various peaks and region of the CV and their significance.

Determine the area and roughness factor of the electrode by Pt oxide region.

**Recommended Texts/References:**

1. Elgrishi, N.; Rountree, K. J.; McCarthy, B. D.; Rountree, E. S.; Eisenhart, T. T.; Dempsey, J. L. A Practical Beginner's Guide to Cyclic Voltammetry, *J. Chem. Educ.***2018**, *95*, *2*, 197–206.

2. B. D. Khosla, V. C. Garg, A. Gulati, Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
3. Field, R. J.; Schneider, F. W. Oscillating Chemical Reactions and Nonlinear Dynamics, *J. Chem. Educ.***1989**, *66*, *3*, 195–204.

**DISCIPLINE SPECIFIC ELECTIVE COURSE-V (DSE-V):**

**Title: Fundamentals of Solid-State and Materials Chemistry (DSE-V, Semester-VIII, 30 Lectures)**

| Course title & Code | Credits | Credit distribution of the Course | | | Eligibility criteria | Pre-requisite of the course (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Fundamentals of Solid-State and Materials Chemistry (DSE-V, Semester-VIII, 30 Lectures) | 04 | 02 | --- | 02 | Class 12th with Physics, Chemistry, Mathematics | --- |

**Course Objectives:**

- To introduce solid-state and wet chemical synthesis methods, and basics of nanomaterials.
- To explain electronic properties of solids using band theory.
- To understand crystal structures, symmetry, and structure determination via diffraction techniques.
- To use thermal and spectroscopic techniques to characterize materials.
- To explore magnetic properties and structure via electron and atomic force microscopy.

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

- Apply solid-state and chemical synthesis methods to create nanomaterials.
- Interpret band structures and explain properties of metals, insulators, and semiconductors.
- Analyze crystallographic data using symmetry concepts and X-ray/electron diffraction.
- Characterize materials using TGA, DSC, UV-Vis, FTIR, PL, and NMR.
- Evaluate magnetic ordering and interpret SEM, TEM, and AFM data.

**Course Contents (Theory):** **Credit: 2 (30 lectures)**

**Unit I: Materials Synthesis and Nanochemistry (6 lectures)**

Solid state reaction and wet chemical synthetic routes, Top down and bottom-up approach to prepare different kinds of nanomaterials, Fundamental concept of nanoscience including quantum confinement effect, Examples: ZnO, $TiO_2$, Ag nanoparticles.

**Init II: Structure and Bonding in Solids (6 lectures)**

Fundamentals of lattice including Bravais Lattices, crystal's direction and planes, symmetry operations and symmetry elements, point group, space group and crystal structures, Miller indices, Types of closed packed structures, Factors which influence crystal structures,Introduction to band theory. Metals, insulators and semiconductors, Electronic structure, k-space and Brillouin zones (qualitative).

**Unit III: Structure Determination by Diffraction (6 lectures)**

Bragg condition and Bragg method, Laue method, PXRD: principles and instrumentation, Crystallite size (Scherrer) and Williamson-Hall method to determine lattice strains from diffraction patterns, Basics of Single Crystal X-ray diffractometer (SCXRD), electron and neutron diffraction.

**Unit IV- Spectroscopy and Thermal Analysis (6 lectures)**

UV-Visible, FTIR, Photoluminescence (PL) and NMR techniques to understand materials properties, Thermogravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC), principles and interpretation, Examples: thermal decomposition, phase changes.

**Unit V: Advanced Characterization and Magnetic Properties (6 lectures)**

Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Atomic Force Microscope (AFM): working principles and applications, Magnetic behaviour: Curie and Curie-Weiss laws, magnetic ordering, exchange interactions, Hysteresis, anisotropy, paramagnetism, ferromagnetism, ferrimagnetism, antiferromagnetism.

**Recommended Texts/References:**

1. H. V. Keer, Principles of the Solid State, Wiley Eastern.

2. W. D. Callister, Materials Science and Engineering, Wiley.
3. C. N. R. Rao, Nanomaterials Chemistry: Recent Developments and New Directions, Wiley-VCH.
4. R. S. Drago, Physical Methods in Chemistry, Saunders College.
5. Ray Egerton, Physical Principles of Electron Microscopy, Springer.
6. Principles of Fluorescence Spectroscopy by Joseph R Lakowicz
7. Fundamentals of Molecular Spectroscopy by C. N. Banwell
8. Introduction to Molecular Spectroscopy, G. M. Borrow, McGraw Hill.


**Supplementary reading**


1. Ashcroft & Mermin, Solid State Physics, Saunders College


**Laboratory Exercises (Practical)(atleast 10): Credit: 2**

**Hands-on experiment**

1. Synthesis of oxide nanomaterials (e.g., ZnO, $TiO_2$) using solid-state or sol-gel methods.
2. Preparation of semiconducting CdSe, ZnSe, $In_2S_3$ (any of one) nanomaterials by any soft chemical approach (emulsion based, co-precipitation etc.).
3. Preparation of metal nanoparticles (e.g., Ag, Cu, or Ni) using standard reduction and capping agents.
4. Studying photocatalytic degradation of environmentally pollutant dye (Crystal Violet, Rhodamine B, methyl orange etc.) by any semiconducting ($In_2S_3$, CdSe, ZnO- any one) or metallic nanoparticles under visible light irradiation and using UV-Visible spectrophotometer.
5. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system).
6. Determination of glass transition temperature of a given salt (e.g. $CaCl_2$) conductometrically.
7. Understanding the differences of functional groups by FTIR analysis of different organic compounds (For example, acids, carbonyls, esters, phenolic OH groups etc.).
8. Determination of band gap of a semiconducting nanoparticle (in solution) using UV-visible spectrophotometer.
9. Determination of band gap of a semiconducting nanoparticle (in solid) using UV-visible spectrophotometer (DRS mode).

**Analysis of Compounds/Sample with pre-recorded spectra/diffraction patterns and images subject to availability of instruments**

1. Measurement and interpretation of different spectra from UV-Vis, IR and NMR using organic, inorganic compounds and molecules. [At least 6 spectra (two from each category) to be provided to students for analysis].
2. Analysis of diffraction pattern obtained from Powder X-ray diffractometer etc (calculation of crystallite size using Scherer equation and lattice strain calculation using Williamson-Hall equation etc). [At least two diffraction patterns of known sample can be provided to students for analysis]
3. Thermogravimetric analysis of compound, molecules etc.
4. Structural analysis using SEM images, EDX analysis of known samples. Students can be provided SEM images and others for analysis.
5. Calculation of particle sizes, aspect ratio from low magnification TEM images of known samples and lattice plane/d spacing calculations from HRTEM images.
6. Facility (PXRD, SCXRD, TEM, SEM and NMR) visits of the students.

**Recommended Texts/References:**


1. B.D. Khosla, V.C. Garg and Adarsh Gulati, Senior Practical Physical Chemistry, R. Chand & Co.
2. J.N. Gurtu, Advanced Physical Chemistry Experiments, Pragati Prakashan.
3. G.N. Mukherjee, University Handbook of Undergraduate Chemistry Experiments, Univ. of Calcutta.
4. Ian M. Watt, The Principles and Practice of Electron Microscopy.
5. Ray F. Egerton, Physical Principles of Electron Microscopy – An Introduction to SEM, TEM and AFM.
6. Yoshio Waseda et al., X-ray Diffraction Crystallography: Introduction, Examples and Solved Problems.
7. Journal articles and datasets from ACS, RSC, Elsevier, as applicable (Ind. Eng. Chem. Res. 2014, 53, 3131−3139; ChemSusChem 2011, 4, 1796−1804; ACS Appl. Mater. Interfaces 2017, 9, 11651−11661; Journal of Luminescence 2007, 124, 327–332)

**DISCIPLINE SPECIFIC ELECTIVE COURSE-VI (DSE-VI):**

**Title: Machine Learning and Artificial Intelligence in Chemistry (DSE-VI, Semester-VIII, 30 Lectures)**

| Course title & Code | Credits | Credit distribution of the course | | | Eligibility criteria | Pre-requisite of the course (if any) |
|---|---|---|---|---|---|---|
| | | Lecture | Tutorial | Practical/ Practice | | |
| Machine Learning and Artificial Intelligence in Chemistry(DSE-VI, Semester-VIII, 30 Lectures) | 04 | 02 | --- | 02 | Class 12th with Physics, Chemistry, Mathematics | --- |

**Course Objectives**

- To develop a fundamental understanding of ML/AI, including their basic concepts and different types of learning
- To become familiar with the basic mathematical foundations of ML
- To understand the principles of ML/AI as applied to chemistry.
- To explore the applications of ML/AI in molecular modeling, drug discovery, quantum-mechanical calculations, catalysis, materials design, etc.
- To gain hands-on experience in implementing ML/AI algorithms and tools in solving chemical problems.

**Learning Outcome**

After completion of this course, learners will be able to-

- Understand core ML/AI principles, including data preprocessing, model training, evaluation, and types of learning.
- Implement and assess ML/AI models (regression, classification, neural networks) for chemistry problems.
- Apply ML/AI to chemical tasks like property prediction, reaction mechanisms, and spectroscopy.
- Integrate ML/AI with quantum chemistry to improve computational efficiency.

**Course Contents (Theory)** **Credit: 2 (30 lectures)**

**Unit I: Introduction to ML/AI in Chemistry(6 lectures)**

Overview of Machine Learning (ML) and Artificial Intelligence (AI). Data pre-processing, model selection, training, and evaluation. Types of learning: Supervised and unsupervised learning. Chemistry-specific challenges in applying AI/ML.

**Unit II: Mathematics for ML/AI(6 lectures)**

Linear Algebra: Vector and Matrix Dot Product, Probability Theory: Random Variables, Bayes Theorem, Conditional Probability, Optimisation: Gradient Descent, First/Second Order Condition.

**Unit III: Machine Learning Models and Techniques(8 lectures)**

Regression and classification models (Linear Regression, SVMs, Decision Trees), Kernel Ridge regression, Neural networks and deep learning, Backpropagation(qualitative), Unsupervised methods: Clustering.

**Unit IV: Applications of ML/AI in Chemistry(10 lectures)**

Application of ML/AI for the discovery of Molecular Design, Materials Sciences and Computational Chemistry; Predicting molecular properties. Prediction of reaction mechanisms and pathways. Binding affinity prediction and molecular docking. QSAR modelling in drug discovery, ML/AI in the design of functional materialsand pharmaceutical chemistry. Predicting spectroscopic properties (IR, NMR, Raman). Accelerating quantum chemistry with ML/AI (e.g., approximating post-HF methods, PES fitting).

**<u>Recommended Texts/References:</u>**


1) Hugh M Cartwright (Ed), Machine Learning in Chemistry: The Impact of Artificial Intelligence, Royal Society of Chemistry; 1st edition (2020)
2) Jon Paul Janet, Heather J. Kulik,Machine Learning in Chemistry, American Chemical Society (2020)
3) Hugh M. Cartwright Applications of Artificial Intelligence in Chemistry, Oxford Chemistry Primers (1994)
4) Pavlo O. Dral,Quantum Chemistry in the Age of Machine Learning, Elsevier - Health Sciences Division (2022)
5) Artificial Intelligence in Chemistry: Current Trends and Future Directions, *J. Chem. Inf. Model.* 2021, 61, 3197−3212
6) A Gentle Introduction to Machine Learning for Chemists: An Undergraduate Workshop Using Python Notebooks for Visualization, Data Processing, Analysis, and Modelling, *J. Chem. Educ.* 2021, 98, 9, 2892–2898
7) The Dawn of Generative Artificial Intelligence in Chemistry Education, *J. Chem. Educ.* 2024, 101, 2957−2959
8) Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems, *Chem. Rev*. 2021, 121, 9816−9872
9) Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis, *J. Med. Chem.* 2020, 63, 8667−8682
10) Artificial Chemical Intelligence: AI for Chemistry and Chemistry for AI by Prof. Pratyush Tiwary, Link: https://www.youtube.com/watch?v=B3wn3C2ANUw


**<u>Laboratory Exercises</u>** <u>(at least 10 practical)</u> **Credit: 2**

1) Fit a polynomial curve using Excel/spreadsheets/colab (linear, quadratic, cubic, quartic, etc) to find a trendline.
2) Perform interpolation and extrapolation on chemical datasets and also find the missing data.
3) Examine extrapolation to predict future values or trends.

4) Build and train a neural network model for molecular property prediction.
5) Running a simple neural network model in machine learning.
6) Fit potential energy surfaces (PES) using neural networks.
7) Use regression models on open-source chemical data (e.g., QM9).
8) Train regression models to predict spectra from structural data.
9) ML pipeline creation in scikit-learn using simple property prediction.
10) Use standard ML python pipelines to train models.
11) Visualization & analysis using tools like Jupyter notebooks/Google Colab.
12) Explore tools and libraries like Numpy, scikit-learn, PyTorch etc. for chemistry research, education, and data analysis.
13) Optional: Explore AI-driven retrosynthesis using IBM RXN or similar platforms (demo only).

**References**:


1. A Gentle Introduction to Machine Learning for Chemists: An Undergraduate Workshop Using Python Notebooks for Visualization, Data Processing, Analysis, and Modeling, *J. Chem. Educ.* 2021, 98, 9, 2892–2898
2. The Dawn of Generative Artificial Intelligence in Chemistry Education, *J. Chem. Educ.* 2024, 101, 2957−2959
3. Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems, *Chem. Rev*. 2021, 121, 9816−9872
4. McQuarrie & Simon,*Physical Chemistry: A Molecular Approach* (for PES concept)
5. a) https://jupyter.org/ b) https://colab.research.google.com/ c) https://www.python.org/ d) https://numpy.org/ e) https://scikit-learn.org/stable/ f) https://pytorch.org/


List of Instruments/Software required for Fourth year for each College

1. UV- Vis Spectrophotometer
2. Digital Photo Fluorometer
3. Polarimeter
4. Table top IR Spectrophotometer
5. ChemDraw
6. HyperChem
7. Access to NMR Spectrophotometer in Department of Chemistry/USIC
8. Rota Evaporator