

**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<br>& Code                                                           | Credits | Credit distribution of the course |          |                        | Eligibility<br>criteria                                     | Pre-<br>requisite<br>of the<br>course<br>(if any) |
|----------------------------------------------------------------------------------|---------|-----------------------------------|----------|------------------------|-------------------------------------------------------------|---------------------------------------------------|
|                                                                                  |         | Lecture                           | Tutorial | Practical/<br>Practice |                                                             |                                                   |
| Coordination Chemistry and Reaction Mechanism (DSC-10: Inorganic Chemistry - IV) | 04      | 03                                | --       | 01                     | Class 12 <sup>th</sup> 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  $\sigma$ -donor,  $\pi$ - acceptor and  $\pi$ - 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  $\text{Cl}^-$

- By Mohr's method
- By Vohlard's method and
- By Fajan's method

#### (B) Complexometric Titrations:

- Complexometric estimation of  $\text{Mg}^{2+}$  /  $\text{Zn}^{2+}$  using EDTA
- Estimation of total hardness of water samples

- (iii) Estimation of  $\text{Ca}^{2+}$  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 Heterocyclic Compounds (DSC-11, Organic Chemistry IV) | 04      | 03                                | --       | 01                  | Class 12 <sup>th</sup> 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**, 9<sup>th</sup> 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**, 7<sup>th</sup> 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**, 1<sup>st</sup> Edition, Berlin, Boston: De Gruyter.
6. Finar, I.L., (2012), **Organic Chemistry** Volume 1, 6<sup>th</sup> 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 <sup>th</sup> 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  $\text{SbO/Sb}_2\text{O}_3$  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<sub>2</sub>SO<sub>4</sub> 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**, 2<sup>nd</sup> Edition, Cengage Learning, India.
3. Castellan, G. W. (2004), **Physical Chemistry**, 4<sup>th</sup> Edition, Narosa.
4. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 3, 6<sup>th</sup> Edition, McGraw Hill Education.
5. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 5, 3<sup>rd</sup> Edition, McGraw Hill Education.
6. Laidler K.J. (2003), **Chemical Kinetics**, 3<sup>rd</sup> 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, 1<sup>st</sup> Edition, McGraw Hill Education.
3. Garland, C. W.; Nibler, J. W.; Shoemaker, D. P. (2003), **Experiments in Physical Chemistry**, 8<sup>th</sup> Edition, McGraw-Hill, New York

**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 <sup>th</sup> 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 hence have 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.  $\pi$ -acceptor behavior of CO (MO diagram of CO to be discussed),  $\pi$ -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  $\pi$ - 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 Fiesher, and Donald A Tarr, **Inorganic Chemistry** 5<sup>th</sup> 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**, 1<sup>st</sup> 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<sup>rd</sup> Edition.
7. Cotton, F.A.; Wilkinson, G.; Gaus, P.L. **Basic Inorganic Chemistry**, 3<sup>rd</sup> Edition, Wiley India.
8. Greenwood, N.N.; Earnshaw, A. (1997), **Chemistry of the Elements**, 2<sup>nd</sup> Edition, Elsevier.
9. Gupta, B. D., Elias, A. J., (2013) **Basic Organometallic Chemistry: Concepts, Syntheses and Applications**, 2<sup>nd</sup> 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 |                                                |                                      |
| <b>Nucleic Acids, Amino Acids, Proteins and Enzymes (DSC-14, Organic Chemistry- V)</b> | <b>04</b> | <b>02</b>                         | <b>--</b> | <b>02</b>           | Class 12 <sup>th</sup> with Physics, Chemistry | <b>--</b>                            |

### 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;  $\alpha$ -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  $\alpha$ -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**, Ninth 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**, Eighth 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 12 <sup>th</sup> 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  $\text{H}_2^+$  and its qualitative extension to  $\text{H}_2$ , Valence bond (VB) treatment of  $\text{H}_2$ , Comparison of LCAO-MO and VB wave functions of  $\text{H}_2$  and their refinements, Qualitative description of LCAO-MO of homonuclear and heteronuclear diatomic molecules- $\text{HF}$  and  $\text{LiH}$ .

#### **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<br><br>(DSC-16: Inorganic Chemistry -VI) | 04      | 02                                | --       | 02                  | Class 12 <sup>th</sup> 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:

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

**(B)**Mixtures should preferably contain one interfering anion, or insoluble component ( $\text{BaSO}_4$ ,  $\text{SrSO}_4$ ,  $\text{PbSO}_4$ ,  $\text{CaF}_2$  or  $\text{Al}_2\text{O}_3$ ) or combination of anions e.g.  $\text{CO}_3^{2-}$  and  $\text{SO}_3^{2-}$ ,  $\text{NO}_2^-$  and  $\text{NO}_3^-$ ,  $\text{Cl}^-$  and  $\text{Br}^-$ ,  $\text{Cl}^-$  and  $\text{I}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$ ,  $\text{NO}_3^-$  and  $\text{Br}^-$ ,  $\text{NO}_3^-$  and  $\text{I}^-$ . 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/<br>Practice |                                                |                                      |
| <b>Polynuclear Hydrocarbons, Photochemistry, Pericyclic Reactions, and Spectroscopy of Organic Compounds (DSC-17, Organic Chemistry-VI)</b> | 04      | 03                                | --       | 01                     | Class 12 <sup>th</sup> 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 Petero Buchi reactions)

## Pericyclic Reactions

Introduction: Types of pericyclic reactions (Electrocyclic, Cycloaddition and Sigmatropic Rearrangements), Symmetry in  $\sigma$  and  $\pi$  molecular orbitals, Frontier Molecular Orbitals.

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

Cycloaddition Reactions:  $[2+2]$  and  $[4+2]$   $\pi$  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.

$^1\text{H}$ -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<sub>2</sub>, AX<sub>3</sub>, A<sub>2</sub>X<sub>3</sub> spin systems, special case of 1-nitropropane.

Applications of IR, UV and  $^1\text{H}$ -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**, 7<sup>th</sup> 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<sup>th</sup> Edition, Wiley.
5. Silverstein R.M. (2005), **Spectrometric Identification of organic compounds**, 7<sup>th</sup> 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**, 4<sup>th</sup> 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/<br>Practice |                                                          |                                      |
| <b>Photochemistry and Spectroscopy (DSC-18, Physical Chemistry VI)</b> | <b>04</b> | <b>02</b>                         | <b>-</b> | <b>02</b>              | <b>Class XII with Physics, Chemistry and Mathematics</b> |                                      |

### 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 ( $\delta$  and  $\tau$ ), 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)  $\text{CuSO}_4$  (ii)  $\text{KMnO}_4$  (iii)  $\text{K}_2\text{Cr}_2\text{O}_7$  in a solution of unknown concentration

2. Determine the concentrations of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  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-phenanthroline.
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  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  (in 0.1 M  $\text{H}_2\text{SO}_4$ ) and determine the  $\lambda_{\text{max}}$  values. Calculate the energies of the two transitions in different units ( $\text{J molecule}^{-1}$ ,  $\text{kJ mol}^{-1}$ ,  $\text{cm}^{-1}$ , eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of  $\text{K}_2\text{Cr}_2\text{O}_7$ .
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

**(C) Analysis of the given vibration-rotation spectrum of  $\text{HCl(g)}$**

**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, 5<sup>th</sup> 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**, 8<sup>th</sup> Edition, McGraw-Hill, New York
3. Kapoor, K.L. (2019), **A Textbook of Physical Chemistry**, Vol.7, 1<sup>st</sup> Edition, McGraw Hill Education.

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