

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 12 th 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, λ_{\max} , chromophores and Auxochromes, bathochromic and hypsochromic shifts, intensity of absorption, factors affecting λ_{\max} values, application of Woodward Rules for calculation of λ_{\max} for the following systems: α , β -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.

^1H -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 ^1H -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