

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 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. 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 Fiesher, and Donald A Tarr, **Inorganic Chemistry** 5th 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**, 1st 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 3rd Edition.
7. Cotton, F.A.; Wilkinson, G.; Gaus, P.L. **Basic Inorganic Chemistry**, 3rd Edition, Wiley India.
8. Greenwood, N.N.; Earnshaw, A. (1997), **Chemistry of the Elements**, 2nd Edition, Elsevier.
9. Gupta, B. D., Elias, A. J., (2013) **Basic Organometallic Chemistry: Concepts, Syntheses and Applications**, 2nd 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**, 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 th 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).

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