COURSES OFFERED BY DEPARTMENT OF CHEMISTRY

B Sc. Life Sciences

Undergraduate Programme of study (with Chemistry as the Major Disciplines)

Semester-wise Distribution of Discipline Specific Core (DSC) Courses

	DISCIPLINE CORE COURSES –02 (4 Credits each)								
SEMESTER	COURSE CODE	NAME OF THE COURSE	CREDITS T=Theory Credits P=Practical Credits						
VII	DSC-19	Chemistry of d- and f- block elements, Advanced Organic Spectroscopy and Elements of Quantum Chemistry	T=3 P=1						
VIII	DSC-20	Organometallic Chemistry and Biocatalysis, Application of Reagents in Organic Synthesis and Crystalline Solids & their Magnetic Properties	T=3 P=1						

DIS	DISCIPLINE SPECIFIC ELECTIVE COURSES – (4 Credits each)									
SEMESTER	COURSE CODE	NAME OF THE COURSE	CREDITS T=Theory Credits P=Practical Credits							
	Common Pool of DSE Courses applicable B.Sc. Physical Sciences and B.Sc. Life S									
	DSE-14	Industrial Chemicals and Environment	T=2 P=2							
	DSE-15	Advanced Stereochemistry	T=2 P=2							
VII	DSE-16	Reactive Intermediates of Organic Chemistry	T=2 P=2							
	DSE-17	Molecular Spectroscopy and Structural Analysis	T=2 P=2							
	DSI	E Course applicable specifically for B.So	c. Life Sciences							
	DSE-18 LS	Nanomedicine and Nanosensing	T=2 P=2							
		Common Pool of DSE Courses applicat B.Sc. Physical Sciences and B.Sc. Life								
	DSE-19	Fundamentals of Natural Products	T=2 P=2							
	DSE-20	Fundamentals of Medicinal Chemistry	T=2 P=2							
VIII	DSE-21	Computational Chemistry	T=2 P=2							
	DSE-22	Machine Learning and Artificial Intelligence in Chemistry*	T=2 P=2							
	DSE	Course applicable specifically for B.Sc	. Life Sciences							
	DSE-23 LS	Bioelectrochemistry	T=2 P=2							
	DSE-24 LS	Nanomaterials and their Biological Applications DSE 22: "Machine Learning and Articles and Arti	T=2 P=2							

^{*} For syllabus content of DSE-22: "Machine Learning and Artificial Intelligence in Chemistry" refer to DSE syllabus of B.Sc. (H) Chemistry.

Note: A student, studying in 4th year of B.Sc. Physical Science/Life Science Programme, desirous of opting any *Discipline Specific Elective* (DSE) Course from progression of DSE courses available in Semester III-VI of the programme, may be allowed to opt the same in the VIIth or VIIIth semester.

Semester VII

DISCIPLINE-SPECIFIC CORE COURSE - 19 (DSC-19): Chemistry of d- and f- block elements, Advanced Organic Spectroscopy and Elements of Quantum Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title &	Credits	Credit di	stribution o	of the course	Eligibility	Pre-
Code		Lecture	Tutorial	Practical/ Practice	criteria	requisite of the course (if any)
Chemistry of d- and f- block elements, Advanced Organic Spectroscopy and Elements of Quantum Chemistry (DSC-19)	04	03	-	01	Class 12 th with Physics, Chemistry	

Course 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 impart the knowledge about synthetic methods and principles of chromatography.
- Understanding spectroscopic techniques and their application in the structural elucidation of organic molecules.
- 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 the hydrogen atom and hydrogen-like atoms.
- To provide an insight into the MO approach of chemical bonding.

Learning outcomes

By studying this course, students will be able to:

- Understand 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.
- Develop understanding on the principles of synthesis of Inorganic compounds and chromatographic separation of metal ions.

- Develop 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.
- Develop an understanding of quantum mechanical operators, quantization, probability distribution, uncertainty principle
- Understand Schrodinger equations for different types of systems
- Analyse different wave functions and probability distribution curves.

UNIT-1: Chemistry of Transition Elements

(15 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

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-2: Spectroscopic Techniques in Organic Chemistry

(15 Hours)

Recapitulation of the Spectroscopic Techniques (UV- VIS, IR, and ¹H NMR)

Carbon-NMR Spectroscopy

Resolution and multiplicity of ¹³C NMR, ¹H-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.

Mass Spectrometry

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.

ESR Spectroscopy

Basic Principles and applications for organic Compounds.

Structure Elucidation

Structure elucidation of Organic Compounds Using UV, IR, NMR, and Mass Spectra.

UNIT -3: Quantum Mechanics: An overview

(6 Hours)

Recapitulation of postulates of quantum mechanics and quantum mechanical operators; Linear and Hermitian operators, commutation rules and Uncertainty principle.

Particle in a 1–D box, quantization of energy levels, zero-point energy, wave functions, probability distribution functions, nodal properties, and qualitative extension to 3-D box (Final Energy expression only) and the concept of degeneracy.

UNIT -4: Quantum Mechanical treatment: Atoms and Molecules (9 Hours)

Vibrational and Rotational Motion: Schrödinger equation of a linear harmonic oscillator and brief qualitative discussion of its results. Schrödinger equation of a rigid rotator and brief qualitative discussion of its results.

Qualitative treatment of hydrogen atom; setting up of Schrödinger equation in spherical polar coordinates, radial part and quantization of energy (only final energy expression). Qualitative idea of indistinguishability of the electrons and their intrinsic spin, spatial and spin wavefunctions, Pauli's Exclusion principle.

Linear Combination of Atomic Orbitals (LCAO), salient features of MO theory and setting up of wavefunction of H_2 molecule.

Practical: Credits: 01

(Laboratory periods: 15 classes of 2 hours each)

PART A: INORGANIC CHEMISTRY

Inorganic Preparations

- 1. Potassium aluminium sulphate KAl(SO₄)₂.12H₂O (potash alum) or Potassium chromium sulphate KCr(SO₄)₂.12H₂O (chrome alum).
- 2. Manganese phosphate and
- 3. Sodium peroxoborate

Paper chromatographic separation of following metal ions (minimum two exercise to be done):

- 4. Ni(II) and Co(II)
- 5. Cu(II) and Cd(II)
- 6. Fe(III) and Al(III)

PART B: ORGANIC CHEMISTRY

(Spectra to be provided wherever required)

- 7. Diels-Alder reaction between maleic anhydride and anthracene and identification of the product using IR and NMR Spectroscopy.
- 8. Knoevenagel condensation between aromatic aldehydes (benzaldehyde/p-nitrobenzaldehyde) and active methylene compounds (malononitrile/ethyl cyanoacetate/ diethylmalonate) and identification of the product using IR and NMR Spectroscopy.
- 9. Differentiate between maleic and fumaric acid solutions by UV spectroscopy.
- 10. Demonstration of the separation of the mixture of *p*-nitrophenol and *o*-nitrophenol by column chromatography and their characterization by melting point and spectroscopic techniques.

PART C: PHYSICAL CHEMISTRY

- 11. Plot the radial wavefunctions and probability distribution for H atom's 1s, 2s, 2p orbitals using software, i.e. MS-EXCEL.
- 12. (i) 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 correlating them with the correspondence principle.
 - (ii) Calculation of the bond length of conjugated dye molecules (i.e., cyanine/β-carotene) using a particle in 1D box model using MS-EXCEL.

Hands-on/Instruction Mode:

- 13. (i) Carry out the calculation of various average values $(\langle x \rangle, \langle p \rangle, \langle x^2 \rangle)$ and $\langle p^2 \rangle$ for the simple harmonic oscillator.
 - (ii) Setting up of Schrödinger equation of Many-electron atoms and cite limitations to carry out an exact solution of the problem.
- 14. Demonstrate the variational treatment of the hydrogen molecule ion and also exhibit Valence bond and Molecular orbital (LCAO) treatment of the hydrogen molecule.

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. 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. S. K. Ghuman, A. Sakthivel, D. T. Masram, M. Sathiyendiran, (2017) Electronic and Magnetic properties of transition and inner transition elements and their complexes, Nova Science Publishers, New York.
- 9. Chandrashekhar, V. (2005), Inorganic and Organometallic Polymers, 5th Edition, Springer Publications.
- 10. Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (1991).
- 11. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. Spectroscopic Identification of Organic Compounds. John Wiley & Sons (1981).
- 12. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. Introduction to Spectroscopy. Cengage Learning (2014).
- 13. Organic Structures from spectra; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., 2007
- 14. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, McGraw Hill Education, Vol 4, 5th Edition, McGraw Hill Education.
- 15. Bakhshi, A. K. & Thakral P., Quantum Chemistry Simplified Vidyavani Foundation: New Delhi (2025).
- 16. House, J.E. (2004), Fundamentals of Quantum Chemistry, 2nd Edition, Elsevier.
- 17. McQuarrie, D.A. (2016), Quantum Chemistry, Viva Books.

- 18. Atkins, P.W.; Paula, J.de. (2014), Atkin's Physical Chemistry Ed., 10th Edition, Oxford University Press.
- 19. Atkins, P.W.; Friedman, R. (2010), Molecular Quantum Mechanics, 5th Edition, Oxford University Press.

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.
- 5. Vogel, A. I. (2012). Quantitative Organic Analysis, Part 3, Pearson Education.
- 6. Mann, F. G., Saunders, B.C. (2009), Practical Organic Chemistry, Pearson Education.
- 7. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A. R. (2012), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
- 8. Ahluwalia, V.K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
- 9. 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.
- 10. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, McGraw Hill Education, Vol 4, 5th Edition, McGraw Hill Education.
- 11. McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books(2008).
- 12. Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
- 13. Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- 14. Yates, P. Chemical Calculations. 2nd Ed. CRC Press (2007).
- 15. Levie, R. de, How to use Excel in analytical chemistry and in general scientific ata analysis, Cambridge Univ. Press (2001) 487 pages.
- 16. Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985).

Semester VIII

DISCIPLINE SPECIFIC CORE COURSE - 20 (DSC-20):

Organometallic Chemistry and Bio- catalysis, Application of Reagents in Organic Synthesis and Crystalline Solids & their Magnetic Properties

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit	distribution	on of the	Eligibility	Pre-
			course		criteria	requisite
		Lecture	Tutorial	Practical/		of the
				Practice		course
						(if any)
Organometallic	04	03		01	Class 12th	
Chemistry and Bio-					with	
catalysis, Application					Physics,	
of Reagents in Organic Synthesis and					Chemistry	
Crystalline Solids &						
their Magnetic						
Properties						
(DSC-20)						

Course Objectives

The objectives of this course are as follows:

- To imparts basic knowledge of Organometallic compounds and catalysis,
- To enrich students with the knowledge of various types of bonding and structure of organometallic compounds and biocatalysts.
- To impart the theoretical and practical knowledge of catalysts with the view of their industrial applications.
- To facilitate chemical transformations by providing the necessary conditions and catalysis.
- To analyze different crystal systems and understand their properties.
- To study Curie's and Curie-Weiss law and its application to paramagnetic and ferromagnetic materials, respectively.
- To understand the principles of powder-XRD and structural analysis of solids.

Learning outcomes

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

- Understand the role of catalyst in industrial applications.
- Gain sound knowledge of various types of catalyst.
- Get skilled in the scientific method of planning, developing, conducting, reviewing and reporting experiments.

- Get skilled concepts of industrial catalysis which will help them to explore new innovative areas of research
- Understand various reducing agents, oxidizing agents, and their applications in organic synthesis.
- Understand the conversion of specific functional groups without affecting others and maximize yields and selectivity for the desired products
- Analyze the distingtion between lattice, unit cell, and the 14 Bravais lattices, and understand their symmetry and properties.
- Interpret XRD patterns of NaCl, CsCl, and KCl to deduce structural information.
- Understand the Curie-Weiss law and its application to ferromagnetic materials.
- Interpret data obtained from instrumental techniques for structural analysis of crystalline solids.

UNIT-1: Organometallic Chemistry and Biocatalysis

(15 Hours)

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, π -acceptor behaviour of carbon monoxide (MO diagram of CO to be discussed), synergic effect and use of infrared spectroscopy data to explain the extent of back bonding. Bio-organometallic chemistry: Conjugates of ferrocene with biomolecules such as amino acid and protein, and their applications. Organometallic complexes as radiopharmaceuticals.

Key aspects of Bio-catalysis, Variables affecting bio-catalysis such as temperature, pH, solvent etc., Enzyme catalyzed reactions and their Kinetics. Detailed study of biocatalyst in the metabolism of Hydrogen, carbon, and sulfur. Nanobiocatalysis.

UNIT- 2: Synthesis and Applications of Reagents in Organic Synthesis (15 Hours)

Synthesis and applications of BuLi, Grignard, organoaluminium, and organozinc reagents.

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, KMnO₄, PCC, OsO₄, CrO₃, K₂Cr₂O₇.

Applications of hydroboration (reductions, oxidations, and carbonylation): Diborane, 9-BBN.

UNIT- 3: Crystalline Solids

(11Hours)

Classification and characteristics of crystalline solids, seven crystal systems. Fundamentals of lattice, unit cell and fourteen Bravais lattices. Types of closed-packed structures. Elementary idea of symmetry. Crystal's direction and planes, Miller indices. X-ray diffraction, Bragg's law. PXRD diffraction pattern of NaCl, CsCl, and KCl,

UNIT -4: Magnetic Properties of Solids

(4 Hours)

Magnetic moment, Curie law, Curie-Weiss law, mechanism of magnetic ordering, exchange Interaction, domain theory, hysteresis, anisotropy, paramagnetism, ferromagnetism, ferrimagnetism, antiferromagnetism.

Practicals: Credits: 01

(Laboratory periods: 15 classes of 2 hours each)

PART A: INORGANIC CHEMISTRY

- 1. Synthesis of "Zeolite A" catalyst.
- 2. Zeolite Hydrogen-Y or dil.HC1/dil.H₂SO₄ as a Catalyst for the Preparation of an Ester.
- 3. Catalytic Synthesis of biaryl.
- 4. Catalytic Transfer Hydrogenation of Castor Oil

PART B: ORGANIC CHEMISTRY

Identification of the product based on Melting point and spectroscopic techniques (IR, ¹HNMR, and ¹³C NMR spectroscopy, data to be provided).

- 5. Synthesis of 1,2,3,4-tetrahydrocarbazole from cyclohexanone.
- 6. Reduction of *p*-nitrobenzaldehyde using NaBH₄
- 7. Synthesis of 2,3-diphenylquinoxaline from benzil and *ortho*-phenylenediamine.
- 8. Oxidation of benzyl alcohol by KMnO₄.

PART C: PHYSICAL CHEMISTRY

- 9. Analysis of diffraction pattern obtained from Powder X-ray diffractometer. Identifying crystal phase, diffraction peaks with lattice planes for a given compound.
- 10. Analysis of p-XRD data of a given set of Metals/ compounds* (Ag/Au/Cu/NaCl/CsCl) and confirmation of the type of the cubic system corresponding to given species.
- 11. Determination of approximate crystallite size using the measured PXRD pattern of a known inorganic compound i.e. TiO₂, ZnO etc by employing Scherer equation.
- 12. Determination of lattice strain using Williamson-Hall equation and from the measured PXRD pattern of a known inorganic compound for example, TiO₂, ZnO etc.*

*[Diffraction patterns of known sample along with Standard JCPDS file (JCPDS: Joint Committee for Powder Diffraction Studies) be provided to students for analysis]

Essential/recommended readings

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. Cotton, F.A.; Wilkinson, G. (1999), Advanced Inorganic Chemistry, Wiley-VCR.
- 3. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), Inorganic Chemistry, 5th Edition, Pearson.
- 4. Jens Hagen (2015) Industrial Catalysis: A Practical Approach Wiley VCR Verlag GmbH&Co
- 5. Gérard Jaouen, (2006) Bioorganometallics, Wiley-VCH Verlag GmbH & Co.
- 6. Carruthers, W. Modern Methods of Organic Synthesis. Cambridge University Press (1996).
- 7. Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).

- 8. Jonathan Clayden, Nick Greeves, Stuart Warren. Organic Chemistry. Oxford. (2000)
- 9. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol 1, 5th Edition, Mc Graw Hill Education.
- 10. Levine I.N. (2009), Physical Chemistry 6th Edition, Mc Graw Hill Education.
- 11. Pillai S.O., (2022) Solid State Physics 6th Edition, New Age International Publishers.
- 12. Chakrabarty, (2022) D. K., Solid State Chemistry, 2nd Edition, New Age International Publishers.
- 13. West, A.R., (2022), Solid State Chemistry and its Applications, 2nd Edition, Wiley Inc.
- 14. Callister W. D., (2018) Materials Science and Engineering: An Introduction, 10th Edition, Willey Inc.
- 15. Keer H. V., (Reprint 2005), Principles of the Solid State, New Age International Publishers.

Practical:

- 1. Williams, D. J.; Huck, B. E.; Wilkinson, A. P. First-Year Undergraduate Laboratory Experiments with Zeolites Chem. Educator 2002, 7, 33-36.
- 2. Coker, E. N.; Davis, P. J.; Experiments with Zeolites at the Secondary-School Level: Experience from The Netherlands Journal of Chemical Education 1999, 76, 10, 1417.
- 3. Hanson RW. Catalytic transfer hydogenation reactions for undergraduate practical programs. J Chem Educ. 2009, 74, 430.
- 4. Alwaseem H, Donahue CJ, Marincean S. Catalytic transfer hydrogenation of castor oil. J Chem. Educ. 2014; 91, 575-8.
- 5. Ahluwalia, V. K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
- 6. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
- 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
- 9. Cullity, B. D. (2001) Elements of X-ray Diffraction, 3rd ed.; Prentice Hall.
- 10. Hammond, C. (2015) *The Basics of Crystallography and Diffraction*, 4th ed.; Oxford University Press.
- 11. Snyder, R. L. (1996) Jenkins, R. Introduction to X-ray Diffractometry; Wiley: New York.
- 12. Hulien M.L., Lekse J.W., Rosmus K. A., Devlin K. P., Glenn J.R., Wisneski S. D., Wildfong P., Lake C. H., MacNeil J. H.Aitken J. A., An Inquiry-Based Project Focused on the X-ray Powder Diffraction Analysis of Common Household Solids, *J. Chem. Educ.* 2015, 92, 12, 2152-2156.
- 13. Evans J. S. O., Evans I.R., Structure Analysis from Powder Diffraction Data: Rietveld Refinement in Excel, *J. Chem. Educ.* 2021, *98*, *2*, *495-505*.
- 14. https://www.icdd.com/ (International Centre for Diffraction Data)

SEMESTER VII

Common Pool of Discipline Specific Elective Courses applicable for both B.Sc. Life Sciences and B.Sc. Physical Sciences

DISCIPLINE SPECIFIC ELECTIVE COURSE – 14 (DSE-14):

Industrial Chemicals and Environment

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title &	Credits	Credit d	Credit distribution of the course			Pre-requisite
Code		Lecture	Tutorial	Practical/	criteria	of the course
				Practice		(if any)
	04	02		02	Class12 th	-
Industrial					with	
Chemicals and					Physics,	
Environment					Chemistry	
(DSE-14)					Biology	

Course Objectives

The objectives of this course are as follows:

The objective of this course is to make students aware about the intricate relationship between industrial processes, the production and use of chemicals, and their profound impact on the environment. Manufacturing, applications, analysis and hazards of the Inorganic Chemicals. Air and Water pollution, control measures for Air and Water Pollutants, Effluents, waste water treatment and Environment.

Learning Outcomes

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

- Understand manufacturing processes, handling and storage of inorganic chemicals.
- Realize hazardous effects of the inorganic chemicals on human beings and vegetation.
- Understand composition of air, various air pollutants, effects and control measures of air pollutants.
- Understand different sources of water, water quality parameters, impacts of water pollution, industrial effluents and water treatment.

UNIT-1: Inorganic Chemicals:

(8 Hours)

Inorganic Chemicals: Manufacture, applications, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potassium dichromate and potassium permanganate

UNIT- 2: Environment and Its Segments

(4 Hours)

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur. Major regions of atmosphere, chemical and photochemical reactions in atmosphere.

UNIT- 3: Air Pollution and its Effects

(8 Hours)

Air pollutants; types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Major sources of air pollution, Pollution by SO₂, CO₂, CO, NO, H₂S and other foul smelling gases, methods of estimation of CO, NOT, SOA and control procedures, Effects of air pollution on living organisms and vegetation, Greenhouse effect and Global warming, Environmental effects of ozone, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and halogens, Air pollution control, Settling Chambers, Venturi Scrubbers, Cyclones, Electrostatic Precipitators (ESPs).

UNIT-4: Water Pollution

(10 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). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro fertilizer. Water quality parameters for wastewater, industrial water and domestic water.

Practicals: Credits: 02

(Laboratory periods: 15 classes of 4 hours each)

- 1. Determination of dissolved oxygen in water.
- 2. Determination of Chemical Oxygen Demand (COD).
- 3. Determination of Biological Oxygen Demand (BOD).
- 4. Percentage of available chlorine in bleaching powder.
- 5. Measurement of chloride, sulphate and salinity of water samples by simple titration method (AgNO₃ and potassium chromate).
- 6. Estimation of total alkalinity of water samples (CO₃^{2-,} HCO₃⁻) using double titration method.
- 7. Measurement of dissolved CO₂ in water samples.
- 8. Determination of hexavalent Chromium Cr(VI) concentration in tannery wastes/waste water sample using UV-Vis spectrophotometry technique.
- 9. Preparation of borax/ boric acid

Essential/recommended readings Theory:

Theory:

- 1. Manahan, S.E. (2017), Environmental Chemistry, CRC Press
- 2. Buchel, K.H.; Moretto, H.H.; Woditsch, P.(2003), Industrial Inorganic Chemistry, Wiley-VCH.
- 3. De, A.K.(2012), Environmental Chemistry, New Age International Pvt., Ltd.
- 4. Khopkar, S.M.(2010), Environmental Pollution Analysis, New Age International Publisher.

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.

DISCIPLINE SPECIFIC ELECTIVE COURSE - 15 (DSE-15):

Advanced Stereochemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title &	Credits	Credit distribution of the course			Eligibility	Pre-requisite
Code		Lecture	Tutorial	Practical/	criteria	of the course
				Practice		(if any)
	04	02		02	Class12 th	-
Advanced					with	
Stereochemistry					Physics,	
(DSE-15)					Chemistry	

Course Objectives

To provide a comprehensive understanding of molecular symmetry, isomerism, and chirality, including their applications in organic reactions.

Learning outcomes

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

- The basic concept of chirality in molecules due to their spatial arrangement of atoms that leads to chiroptical properties.
- 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.
- That, stereochemistry significantly impacts drug action, biological processes, and chemical reactions, influencing factors like drug efficacy, selectivity, and even the rate of chemical reactions.

UNIT -1: (15 Hours)

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.

UNIT -2: (5 Hours)

Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres.

UNIT-3: (3 Hours)

Asymmetric induction: Cram's, Prelog's, and Felkin-Ahn model.

Unit-4: (7 Hours)

Cyclostereoisomerism: Configurations, conformations and stability of cyclohexanes (di-, and tri-substituted), cyclohexenes, cyclohexanones, decalin.

Applications of ORD and CD to Stereochemical Problems

Practicals: Credits: 02

(Laboratory periods:15 classes of 4 hours each)

- 1. E/Z and Cis-Trans Isomerism of 2,3-dimethyl-2-butene by ball and stick models
- 2. Identification of Chiral Centres 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 determining their 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. Proline-catalyzed aldol reaction of cyclohexanone with nitro-substituted benzaldehydes.⁵
- 12. 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

Essential/recommended readings Theory:

- 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

Practical:

- 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 ¹H 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 - 16 (DSE-16): Reactive Intermediates of Organic Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title	Credits	Credit d	istribution	of the course	Eligibility	Pre-requisite
& Code		Lecture	Tutorial	Practical/	criteria	of the course
				Practice		(if any)
	04	02		02	Class 12th	-
Reactive					with	
Intermediates					Physics,	
of Organic					Chemistry	
Chemistry						
(DSE-16)						

Course Objectives

The objectives of this course are as follows:

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.

Learning outcomes

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

- Understand the structure-reactivity pattern of reactive intermediates involved in organic reactions.
- Analyse the mechanism of organic reactions involving reactive intermediates and apply these reactions in organic synthesis

Unit 1: Carbocations and Carbanions

(11 Hours)

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.

Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications.

Unit 2: Carbenes and Nitrenes

(12 Hours)

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.

Structure of nitrene, generation and reactions of nitrene and related electron-deficient nitrogen intermediates, Curtius, Hoffmann, Schmidt, Beckmann rearrangement reactions.

Unit 3: Ylides (2 Hours)

Chemistry of Phosphorus and Sulfur ylides – Wittig and related reactions, Peterson olefination.

Unit 4: Radicals (5 Hours)

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.

Practicals: Credits: 02

(Laboratory periods:15 classes of 4 hours each)

(Experiments 1 and 2 are compulsory)

1. Separation, purification, and identification of binary mixtures of organic compounds (neutral and acidic; neutral and basic) using chemical methods and preparation of a suitable crystalline derivative for both the components.

2. Two-step synthesis

2.1 To carry out the synthesis of triacetoxybenzene

- Step 1: Synthesis of p-benzoquinone from hydroquinone using KBrO₃ and
- Step 2: Synthesis of Triacetoxybenzene from p-benzoquinone.

2.2 To carry out the 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 To carry out the synthesis of benzopinacolone

- Step 1: Synthesis of benzopinacol from benzophenone
- Step 2: Synthesis of benzopinacolone from benzopinacol via pinacol-pinacolone rearrangement.

Essential/recommended readings

Theory:

- 1. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5thedition, 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.

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 ELECTIVE COURSE – 17 (DSE-17):

Molecular Spectroscopy and Structural Analysis

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title	Credits	Credit d	istribution	of the course	Eligibility	Pre-requisite
& Code		Lecture	Tutorial	Practical/	criteria	of the course
				Practice		(if any)
	04	02		02	Class 12th	
Molecular Spectroscopy and Structural Analysis (DSE-17)					with Physics, Chemistry	

Course Objectives

The objectives of this course are as follows:

- To introduce the fundamental principles of spectroscopy, including the characterization of electromagnetic radiation and the Born-Oppenheimer approximation.
- To explore transition dipole moments and selection rules, with emphasis on symmetry ideas and time-dependent perturbation in spectroscopic processes.
- To analyze the principles and instrumentation of Raman spectroscopy and understand vibrational and rotational Raman spectra.
- To study the spectroscopic techniques for structural analysis i.e. AFM, SEM, and TEM.

Learning outcomes

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

- Understand the principles of electromagnetic radiation and fundamental spectroscopic concepts, including the Born-Oppenheimer approximation and time-dependent perturbation.
- Analyze Raman spectroscopy and deduce the structure of molecules using vibrational and rotational Raman spectra.
- Describe the Atomic spectra, the spin and orbital selection rules, spectra of complex atoms and basic principles of atomic photoelectron spectroscopy.
- Exhibit their understanding of theoretical basis of rotational, vibrational, raman and NMR spectroscopy.
- Have an insight into spectroscopic techniques for Structural Analysis i.e. SEM, TEM and AFM.

Unit 1: Basic Concepts of Spectroscopy and Atomic Spectra (8 Hours)

Spectroscopy and its importance in chemistry. Heisenberg Uncertainty Principal; Link between spectroscopy and quantum chemistry. Types of spectroscopy. Time dependent perturbation. Einstein coefficients. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry considerations.

Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials. Spectra of complex atoms. Zeeman and Stark effects, Atomic photoelectron spectroscopy (Qualitative Discussion only).

Unit 2: Rotational, Vibrational and Raman Spectroscopy

(14 Hours)

Rotational spectroscopy Determination of bond lengths and atomic mass. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules.

Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules. Anharmonic oscillator; Morse potential. Overtones and hot-bands. Dissociation energies from vibrational data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation. Nuclear spin effect. Symmetry of normal coordinates.

Stokes and anti-Stokes lines. Polarizability ellipsoids. Rotational and vibrational Raman spectroscopy. Selection rules. Rule of Mutual Exclusion. Polarization of Raman lines.

Unit 3: NMR spectroscopy:

(5 Hours)

Larmor precession. Mechanisms of spin-spin and spin-lattice relaxations and quantitative treatment of relaxation. Quantum mechanical treatment of the AB system. Selection rules and relative intensities of lines.

Unit 4: Microscopic Techniques for Structural Analysis

(3 Hours)

Elementary idea of Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), and Atomic Force Microscope (AFM) for structural analysis.

Practicals: Credits: 02

(Laboratory periods:15 classes of 4 hours each)

- 1. Analyse UV-Vis absorption spectra of conjugated systems (e.g., β -carotene) and determine the HOMO-LUMO gap.
- 2. Study the effect of structure on the UV spectra of organic compounds.
- 3. 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.
- 4. Find the stoichiometry of the charge transfer (CT) complex formed between thiocyanate ions and iron (III) by Job's method of continuous variation.
- 5. Record the UV spectra of a weak acid (α -naphthol) at different pH and determine the dissociation constant in the ground state.

Hands-on/ Demonstration/Instruction Mode: Demonstration/Discussion of working principle/Hands-on with substantial literature analysis/Laboratory exercise

- 6. 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.
- 7. Perform IR and Raman spectroscopy on symmetrical molecules (e.g., CS₂, CO₂) and analyze the mutual exclusion principle.

- 8. Calculate the force constant (k) of diatomic molecules (e.g., HCl, N₂) from IR spectra.
- 9. Create a calibration curve and use it to determine the concentration of a fluorophore in unknown samples.
- 10. Simulate and analyze rotational spectra of rigid rotor molecules.
- 11. Measure absorbance vs. time data to study the kinetics of fast photochemical reactions (using Time-Resolved Absorption Spectroscopy for Reaction Kinetics).
- 12. Resolve and assign vibrational fine structure in the UV-Vis spectrum of iodine vapor.

Essential/recommended readings

Theory:

- 1. Hollas. J. M., *Modern Spectroscopy* 4th Ed., John Wiley & Sons (2004).
- 2. Satyanarayana, D. N., *Handbook of Molecular Spectroscopy: From radio waves to gamma rays*, I.K. International Publishing House, New Delhi (2015).
- 3. Kakkar, R., Atomic & Molecular Spectroscopy, Cambridge University Press (2015).
- 4. Brand, J. C. D. & Speakman, J. C. *Molecular Structure: The Physical Approach* 2nd Ed., Edward Arnold: London (1975).
- 5. Chang, R. Basic Principles of Spectroscopy McGraw-Hill, New York, N.Y. (1970).
- 6. Moore, W. J. Physical Chemistry 4th Ed. Prentice-Hall (1972).
- 7. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol 1, 1st Edition, Mc Graw Hill Education.

Practical:

- 1. B. D. Khosla, V. C. Garg, A. Gulati, Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
- 2. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy.
- 3. A. Findlay, B.P. Levitt, J.A. Kitchener, Experimental Physical Chemistry.
- 4. Donald A. McQuarrie and John D. Simon, Physical Chemistry: A Molecular Approach.
- 5. J. Michael Hollas, Modern Spectroscopy.
- 6. Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis.
- 7. Jeanne L. McHale, Molecular Spectroscopy.
- 8. Donald L. Pavia, Gary M. Lampman, George S. Kriz, Introduction to Spectroscopy.
- 9. Gurdeep R. Chatwal and Sham K. Anand, Spectroscopy: Atomic and Molecular.
- 10. Peter Atkins and Ronald Friedman, Molecular Quantum Mechanics.

Discipline Specific Courses Applicable Specifically for B.Sc. Life Sciences

DISCIPLINE SPECIFIC ELECTIVE COURSE – 18 LS (DSE-18 LS): Nanomedicine and Nanosensing

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title	Credits	Credit distribution of the course			Eligibility	Pre-requisite
& Code		Lecture Tutorial Practical/		criteria	of the course	
				Practice		(if any)
Nanomedicine	04	02		02	Class 12 th	
and					with	
Nanosensing					Physics,	
(DSE-18 LS)					Chemistry	

Course Objectives

The objectives of this course are as follows:

- To discuss the various nanomaterials to be used as drug delivery systems.
- To develop an understanding of living system interaction of nanomaterials
- To enable learners to have an insight into the field of nanodiagnostics.
- To explain nature of nanomaterials as nanosensors.

Learning outcomes

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

- Demonstrate understanding of the concept of nanomaterial as efficient drug delivery systems.
- Evaluate Living System Interaction of Nanomaterials, thereby, exhibit foray into field of nanodiagnostics.
- Understand basic principle of gas sensing, chemosensing, biosensing, Optical, electrochemical, magnetic sensing using various nanoparticles.
- Perform hands-on laboratory exercise aimed at designing a variety of nanomaterials and their subsequent application in nanomedicine and nanosensing.

Unit 1: Nanomaterial and Drug Delivery - (8 Hours)

Nanomaterials of biological interest: Lipid-, polymer-(PLGA, PVP), inorganic-based (Gold, iron-oxide and silica) and hybrid nanomaterials. Nanomaterials as drug delivery systems. Encapsulation and release of drugs, photosensitizers (porphyrins), DNA, and other active agents i.e. coumarin dyes. Stimuli-responsive drug release.

Unit 2: Living System Interaction of Nanomaterials (7 Hours)

Interaction of nanomaterials with mammalian cells; Endocytosis, phagocytosis, pinocytosis, and other cell-entry mechanisms. Fate of nanoparticles inside cells. In vitro assays: cell viability, ROS determination, biochemical assays, etc.

Unit 3: Nanodiagnostics

(7 Hours)

Nanodiagnostics: Basics of optical imaging, MRI, CT imaging, radioimaging. Nanomaterials (gold nanospheres and nanorods, dye-doped silica nanoparticles) for optical imaging, magnetic resonance imaging, CT imaging, radio-imaging, etc. Structural and Functional imaging. Imageguided drug delivery.

Unit 4: Nanosensing (8 Hours)

Basic principle of gas sensing, chemosensing, biosensing, Optical, electrochemical, magnetic sensing using various nanoparticles (gold nanospheres and nanorods, iron-oxide nanoparticles, nanographene and nanographene oxide). In vitro diagnostics from simple body fluids such as blood and urine. Microfluidic technology for low volume and high throughput sensing.

Practicals: Credits: 02

(Laboratory periods:15 classes of 4 hours each)

<u>Hands-on/Demonstration/ Instruction Mode:</u> Demonstration/ Discussion of working principle/ Hands-on with substantial literature analysis/ Laboratory exercise.

- 1. (i) Synthesis of nanoparticles: Gold nanospheres and nanorods, nanographene, iron-oxide nanoparticles.
 - (ii) Characterization and differentiation of Gold nanospheres and nanorods using spectrophotometric analysis.
- 2. Preparation of PLGA nanoparticles.
- 3. Preparation of liposomes, solid-lipid nanoparticles (SLNs),
- 4. Synthesis of silica and organically modified silica (ormosil) nanoparticles,
- 5. Estimation of loading capacity of Drug/dye and release kinetics study in liposomes, PLGA nanoparticles, SLNs, ormosil nanoparticles, and ZIF-8 nanoscale frameworks (Any one system).
- 6. Comparative reaction kinetics study of dye-degradation (rhodamine-B) using Au/ Ag/ Au-Ag nanoparticles.
- 7. Colorimetric determination of trace amount of metal ions (*Iron or copper*) using gold nanospheres/nanorods.
- 8. LED-light-activated photothermal experiments using gold nanospheres/nanorods using temperature change measurements.
- 9. Determination of protein binding capacity of gold nanoparticles using NMR study.

Essential/recommended readings

Theory:

- 1. Prasad 1. P. N.. Introduction to Nanomedicine and Nanobioengineering. Wiley, 2012.
- 2. Webster. T. J. Nanomedicine Technologies and Application (2 nd Edition) ScienceDirect, 2023.
- 3. Jain. K. K. The Handbook of Nanomedicine. Springer, 2017
- 4. Kulkarni S. K., Nanotechnology: Principles and Practices, Springer Cham, 2014 (978-3-319-09171-6).
- 5. Singh K., Nanoparticle Therapeutics, Academic Press Elsevier, 2021 (978-0-12-820757-4).

- 6. Ratner B. D., Hoffman A. S., Schoen F. J., Lemons J. E., Biomaterials Science, Press Elsevier, 2013 (978-0-12-374626-9)
- 7. Nelson D. L., Cox M., Principles of Biochemistry, WH Freeman, 7th ed. 2017 (978-1319108243)
- 8. Alberts B., Johnson A., Lewis J., Raff M., Roberts K., Walter P., Molecular Biology of the Cell, 4th ed., Garland Science, 2002, 10: 0-8153-3218-1

Practical:

- 1. Prasad P. N.. Introduction to Nanomedicine and Nano-bioengineering. Wiley, 2012.
- 2. Webster. T. J. Nanomedicine Technologies and Application (2 nd Edition) Science Direct, 2023.
- 3. Jain. K. K. The Handbook of Nanomedicine. Springer, 2017
- 4. Kumar C., Hormes J., Leuschner C., Nanofabrication Towards Biomedical Applications, Wiley Vch., 2005 (9783527311156)
- 5. Greco R. S., Prinz F. B., Smith R. L., Nanoscale Technology in Biological Systems, CRC Press, 2004 (9780849319402).
- 6. Perera Y. R., South T.M., Hughes A. C., Parkhurst A. N., Williams O.C., Davidson M. B., Wilks C. A., Misna D. A., Fitzkee N.C., Using NMR spectroscopy to measure protein binding capacity on gold nanoparticles, *J. Chem. Educ.* 2020, *97*, *3*, 820-824.
- 7. Bentley A. K., Farhoud M, Ellis A. B., Lisensky G.C., Nickel A-Marie L, Crone W. C., Template Synthesis and Magnetic Manipulation of Nickel Nanowires, *J. Chem. Educ.* 2005, 82, 5, 765-768.
- 8. Oliveira M. L., Pagung E., Lorenzini L., Neves T.R., Pereira J.R.P., Ferreira S. A. D., Freitas M. B. J.G. de, Moura P. R.G., Lelis M. F. F., Synthesis of Iron Oxide Nanoparticles and their Application in Photo-Fenton Process: An Undergraduate Experiment in Chemistry, *J. Chem. Educ.* 2025, *102*, *1590-1597*.
- 9. How to Characterize 4–90nm Size Gold Nanospheres with Experimental and Simulated UV–Vis and a Single SEM Image, *J. Chem. Educ.* 2023, *100*, *1589-1596*.
- 10. Nedrygailov I, Brien D. O., Monaghan S., Hurley P, Biswas S., Holmes J.D., Nanowood: A Unique Natural Nanomaterial That Can Be Obtained Using Household Chemicals, *J. Chem. Educ.* 2024, *101*, *11*, 4931-4936.

SEMESTER VIII

Discipline Specific Courses (Common Pool) applicable for both B.Sc. Life Sciences and B.Sc. Physical Sciences

DISCIPLINE SPECIFIC ELECTIVE COURSE – 19 (DSE-19) Fundamentals of Natural Products

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit	distribution course	Eligibility criteria	Pre- requisite	
		Lecture	Tutorial	Practical / Practice		of the course (if any)
Fundamentals of Natural Products (DSE-19)	04	02		02	Class 12 th with Physics, Chemistry	

Course Objectives

The objectives of this course are as follows:

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.

Learning outcomes

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

- Understand the scope and significance of natural product chemistry in both historical and modern contexts, particularly its role in drug discovery.
- Analyze and classify major natural product groups-such as alkaloids, terpenoids, flavonoids, phenolics, peptides, glycosides, polyketides, steroids, and hormones-and understand their structures and functions.

Unit 1: Introduction and Classification of Natural Products: (11 Hours)

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.

Alkaloids, Terpenoids, Flavonoids, Phenolics, Peptides and Proteins, Glycosides, Polyketides, Steroids and Hormones. Isoprene rule, mevalonate and non-mevalonate pathways, Shikimic acid pathway.

Unit 2: Isolation and Purification Techniques:

(4 Hours)

Extraction methods (solvent extraction, Soxhlet, maceration, etc.), Chromatographic techniques (TLC, Column, HPLC, GC-MS), Crystallization and distillation techniques, Bioassay-guided fractionation.

Unit 3: Total Synthesis of Natural Products:

(10 Hours)

Artemisinin (Antimalarial); Berberine (anti-inflammatory); Lysergic Acid Diethylamide (Psychedelic drug), and Vitamin B12.

Unit 4: Biosynthesis of Natural Products:

(5 Hours)

Artemisinin, Berberine, and Lysergic Acid Diethylamide (LSD).

Practicals: Credits: 02

(Laboratory periods:15 classes of 4 hours each)

- 1. Isolation of natural products: Isolation of β -carotene from carrots.
- 2. Isolation of natural products: Isolation of limonene from lemon peel/orange peel.
- 3. Isolation of natural products: Isolation of caffeine from tea leaves.
- 4. Isolation of natural products: Isolation of piperene from black pepper.
- 5. Isolation of natural products: Isolation of eugenol from cloves.
- 6. Isolation of protein and carbohydrates from seeds –colour test.
- 7. Synthesis of 7-hydroxy-4-methylcoumarin
- 8. Synthesis of a simple dipeptide(gly-gly) by DCC coupling using N-protected amino acids.
- 9. Synthesis of simple amino acids

Essential/recommended readings

Theory:

- 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)

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 ELECTIVE COURSE – 20 (DSE-20) Fundamentals of Medicinal Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre- requisite
		Lecture	Tutorial	Practical /		of the course
				Practice		(if any)
Fundamentals of	04	02		02	Class 12th	
Medicinal					with Physics,	
Chemistry					Chemistry	
(DSE-20)						

Course Objectives

The objectives of this course are as follows:

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.

Learning outcomes

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

- Understand the development and role of medicinal chemistry, understand the stages of drug discovery, and evaluate drug screening and clinical processes.
- Interpret how stereochemical and physicochemical properties influence drug behavior and efficacy.

Unit 1: Introduction to Medicinal Chemistry and Drug discovery: (15 Hours)

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.

Target identification and validation, Screening of drugs, High throughput screening (HTS), Random and Systematic screening. Structure activity relationship (SAR), Hit identification, and Lead optimization

Unit 2: Pharmacokinetics (ADME):

(5 Hours)

Drug administration/absorption, drug distribution, drug metabolism - Phase 1 and Phase 2, drug excretion, Half-Life of drugs, and Clinical trials.

Unit 3: Representative Synthetic Drugs:

(7 Hours)

Structure, Synthesis, and Therapeutic Value of Representative Drugs: Fluconazole (antifungal), Penicillin (antibiotic), Isoniazid (antibiotic), and Azidothymidine (AZT; anti-HIV).

Practicals: Credits: 02

(Laboratory periods:15 classes of 4 hours each)

- 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.
- 7. Synthesis of Benzocaine, a topical pain reliever.
- 8. Isolation of Caffeine from tea leaves using solvent extraction techniques.
- 9. Estimation of Vitamin C.

Essential/recommended readings

Theory:

- 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)

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 ELECTIVE COURSE - 21 (DSE-21) Computational Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title	Credits	Credit distribution of the course			Eligibility	Pre-requisite
& Code		Lecture Tutorial Practical/ c		criteria	of the course	
				Practice		(if any)
Computational	04	02		02	Class 12th	
Chemistry					with	
(DSE-21)					Physics,	
·					Chemistry	

Course Objectives

The objectives of this course are as follows:

- To introduce the fundamental concepts and theoretical background of computational chemistry.
- To develop an understanding of quantum mechanical, semi-empirical and molecular mechanical methods used in molecular modeling and molecular dynamics.
- To enable learners to perform geometry optimization, energy calculations, and vibrational analysis using computational tools.
- To teach the interpretation of computational results in the context of chemical structure, and reactivity.
- To expose students to various software packages commonly used in computational chemistry
- To provide hands-on experience with setting up, running, and analyzing computational chemistry simulations.

Learning outcomes

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

- Demonstrate a solid understanding of key computational methods such as ab initio, semi-empirical, and molecular mechanical methods.
- Apply computational tools to predict and analyze molecular properties, geometries, and reaction mechanisms.
- Perform and interpret quantum chemical and molecular simulation calculations using standard software packages.
- Evaluate the accuracy and limitations of various computational approaches in relation to experimental data.
- Design and conduct computational experiments to solve problems in chemical research and development.

Unit 1: Fundamentals of Computational Chemistry

(6 Hours)

Conceptual background of computational chemistry and molecular modeling, Z-matrix of simple molecules, Born-Oppenheimer approximation and Potential Energy Surfaces (minima

and maxima), harmonic frequency calculations and intrinsic reaction coordinate. Charge analysis (Milliken. NBO, etc.). Cost and efficiency.

Unit 2: Molecular Mechanics and Molecular Dynamics (12 Hours)

Molecular Mechanics: Force Fields, Non-bonded interactions (van der Waals and electrostatic, hydrogen bonding), Parameterization. The applications of MM, the disadvantages, and the different variants of MM (MM1, MM2, MM3, MM4, AMBER, OPLS, etc).; Molecular Dynamics: Ensembles (microcanonical, canonical, isothermal – isobaric), Concept of periodic box, Ergodic hypothesis. Leapfrog and Verlet Algorithms (qualitative treatment), Typical MD simulations.

Unit 3: Semi-empirical Methods

(3 Hours)

Brief idea of semi-empirical method; CNDO, INDO, MNDO, AM1, PM3.

Unit 4: Quantum Mechanical Methods

(9 Hours)

Brief idea of quantum mechanical methods; HF, MP2, DFT, CC, and CI (conceptual and qualitative discussion only)

Conceptual ideas of Basis sets (STOs and GTOs), diffuse and polarization functions, Basis set superposition error (BSSE), Effective Core Potentials (ECP), and HOMO-LUMO. Awareness of available computational chemistry software.

Practicals: Credits: 02

(Laboratory periods:15 classes of 4 hours each)

- 1. Find the Z-matrix of diatomic (i.e., H₂, HCl), triatomic (i.e., H₂O, HNO, HCN) and tetratomic (i.e., H₂CO, HNO₂, BH₃, cis- and trans-diazene) molecules, etc.
- 2. Determine the optimized geometry of HF, HCl, and HBr molecules and compare the optimized geometrical parameters, formal charges, vibrational frequencies, and dipole moments using AM1, HF, and DFT (using at least three different basis sets).
- 3. Determine the optimized geometry of HF, HCl, and HBr molecules and compare the optimized geometrical parameters, formal charges, vibrational frequencies, and dipole moments by DFT method at least three different basis sets using any suitable method.
- 4. Determine the optimized geometry of H₂O, H₂S, and H₂Se molecules and compare the optimized geometrical parameters, formal charges, vibrational frequencies, and dipole moments by HF, DFT and MP2 methods using at least three different basis sets.
- 5. Calculate and compare the C-C, C=C and C=C bond dissociation energies of ethane, ethylene, and acetylene molecules, respectively, using any suitable method/basis set.
- 6. Calculate and compare the bond dissociation energies of HF, HCl, and HBr molecules using any suitable method/basis set.
- 7. Generate the potential energy surface diagram for the rotational profile of the ethane molecule around the C–C bond.
- 8. Generate the potential energy surface diagram for the rotational profile of the butane molecule around the C₂–C₃ bond
- 9. Determination of Frontier Molecular orbitals of H₂, CO, HF, H₂O, H₂CO and benzene molecules using any suitable method/basis set.

- 10. Determine the activation energy for the isomerization of cis-diazene to trans-diazene by computing the equilibrium geometries and the transition state structure using any suitable method/basis set.
- 11. Calculate the intrinsic reaction coordinate (IRC) for cis-diazene to trans-diazene transformation using any suitable method/basis set.
- 12. Using optimized geometries, calculate the reaction enthalpy at 298 K for the following industrially important reactions (Haber-Bosch process) based on the enthalpies of the involved species: $CH_4 + H_2O \rightarrow CO + 3H_2$
- 13. Calculate formaldehyde/benzene's electronic UV/Visible absorption spectrum.
- 14. Based on the conceptual DFT, calculate the ionization potential (IP), electron affinity (EA), electronegativity, and electron chemical potential of a given set of molecules.
- 15. Study the mechanism of SN_2 reaction between Cl⁻ and CH₃Br involving a Walden inversion computationally.
- 16. Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- 17. Predict the aromaticity of thiophene with respect to benzene by comparing their enthalpies of hydrogenation.
- 18. Arrange 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.
- 19. Compare the basicity of the nitrogen atoms in ammonia, methylamine, dimethylamine, and trimethylamine by comparison of their charges and ESP maps.
- 20. Compare the HXH bond angles for the second-row hydrides (BeH₂, CH₄, NH₃, H₂O) and compare with the results from qualitative MO theory (here, X = Be, C, N and O).
- 21. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).

Note: Minimum 12 exercise to be performed. Any other practical may also be performed as directed by the instructor.

NB: Some suggested free open-source software tools include:

- (a) For visualization and basic tasks: Avogadro, Jmol, RasMol, Molden, IQmol, PyMOL, VMD, MacMolPlt, ArgusLab, ChemCraft (for 150 days) or any other software may be used.
- (b) For calculations and simulations: Avogadro, ArgusLab, Dalton, Ergo, GAMESS, ORCA, NW Chem, MPQC, Psi4, Quantum ESPRESSO, ABINIT, CP2K, TINKER or any other available software may be used.

References:

- 1. C. J. Cramer, *Essentials of Computational Chemistry-Theories and Models*, John Wiley and Sons Ltd., 2nd Ed., 2004.
- 2. F. Jensen, *Introduction to Computational Chemistry*, John Wiley and Sons Ltd., 3rd Ed., 2017.

- 3. Free and open source software for computational chemistry education, S. Lehtola and A.
 - J. Karttune, Comput Mol Sci. (2022); 12, e1610. doi: 10.1002/wcms.1610
- 4. Online manual of
 - a) Gaussian 16, www.gaussian.com
 - b) GAMESS, www.msg.ameslab.gov/gamess
 - c) Q-Chem, https://manual.g-chem.com/latest/
- 5. J. B. Foresman and Æ Frisch, *Exploring Chemistry with Electronic Structure Methods*, 3rd ed., Gaussian, Inc.: Wallingford, CT, 2015.

DISCIPLINE SPECIFIC ELECTIVE COURSE - 22 (DSE-22): Machine Learning and Artificial Intelligence in Chemistry

*For syllabus content of Discipline Specific Elective-22: (DSE-22) "Machine Learning and Artificial Intelligence in Chemistry refer to the pool of DSE courses in 4th year syllabus of **B.Sc. (H) Chemistry**.

Discipline Specific Courses Applicable Specifically for B.Sc. Life Sciences

DISCIPLINE SPECIFIC ELECTIVE COURSE – 23 LS (DSE-23 LS) Bioelectrochemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit	distribution course	on of the	Eligibility criteria	Pre- requisite
		Lecture	Tutorial	Practical / Practice		of the course (if any)
Bioelectro- chemistry (DSE-23 LS)	04	02		02	Class 12 th with Physics, Chemistry	-

Course Objectives

The objectives of this course are as follows:

- To provide a conceptual understanding of the various types of electrodes and the electrochemical processes.
- To equip the students with conceptual understanding of the electrical double layer and Equivalent circuit models of EDL; Gouy-Chapman Model etc.
- To help build an insight into Interfacial Electron Transfer in Biological Systems.
- To provide an understanding of the concept of bio-electrocatalysis and electrochemical communication in biological organisms.

Learning outcomes

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

- Differentiate between different electro systems and account for the electrochemical processes at the electrodes.
- Demonstrate their understanding of the electrical double layer, membrane potential and the concept of interfacial electron transfer in biological systems.
- Exhibit their understanding of Chemical signalling, electrical signalling. Electrochemical mechanisms of the nervous system
- Develop an insight into Bioelectrocatalysis Using Enzymes electrodes.

Unit 1: Electrode and Electrochemical Processes

(8 Hours)

Qualitative conceptual description of working and Counter Electrodes, Reference Electrodes: standard hydrogen electrode (SHE), or normal hydrogen electrode (NHE), saturated calomel electrode (SCE), silver-silver chloride electrode, potential of zero charge, open-circuit potential of the cell, overpotentials.

Faradaic and Nonfaradaic Processes: Ideally polarizable electrode, Capacitance and Charge of an Electrode, supporting electrolyte, Nernst equation, Nernst potential and biological systems.

Description of the Electrical Double Layer: Stern Potential, Zeta potential. Membrane potentials, simplistic theories of membrane potentials, electrical conduction in biological organisms: electronics and protonics.

Unit 2: Electrical Double Layer

(8 Hours)

Description of the Electrical Double Layer: inner and outer compact layer Helmholtz, Stern layer, Diffuse Layer, specifically and non-specifically adsorbed ions, Potential profile across the double-layer region in the absence of specific adsorption of ions, Equivalent circuit models of EDL, Gouy-Chapman Model (Qualitative discussion only)

Brief qualitative discussion of basic principle and application of electrophoeresis, Electrochemical impedance spectroscopy and cyclic voltammetry techniques.

Unit 3: Interfacial Electron Transfer in Biological Systems

(6 Hours)

Electrode kinetics, Butler-Volmer equation, adsorption of proteins onto metals from solution, electron transfer from biomaterials to simple redox ions in solution, theoretical aspects of electron transfer from solid proteins to ions in solution.

Unit 4: Electrochemical Communication and Bio-Electrocatalysis (8 Hours)

Chemical signalling, electrical signalling. Electrochemical mechanisms of the nervous system, theory of the spike potential. Monitoring neurotransmitters in the intact brain and other single-cell studies.

Bio-Electrocatalysis, electrodes carrying enzymes, electrochemical enzyme-catalyzed oxidation of styrene.

Practicals: Credits: 02

(Laboratory periods:15 classes of 4 hours each)

- 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. Effect of ionic strength on reaction rate (persulfate-iodine reaction).
- 3. Potentiometric determination of solubility and solubility product of AgCl(s) in water.
- 4. Potentiometric determination of mean ionic activity coefficient of HCl at different concentrations.
- 5. Potentiometric titration of Phosphoric acid vs NaOH.
- 6. Determination of dissociation constant of acetic acid from its potentiometric titration curve.

<u>Hands-on/Demonstration/ Instruction Mode:</u> Demonstration/ Discussion of working principle/ Hands-on with substantial literature analysis/ Laboratory exercise.

- 7. To measure the Vitamin C content of commercial Orange Juice using Pencil Lead as a working electrode in cyclic voltammetry.
- 8. Synthesis and Cyclic voltammetry study of Nano-wood, prepared using household Chemicals.
- 9. 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 $NaNO_3$)
- 10. 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 $Fe(NH_4)_2 (SO_4)_2 + Fe(NH_4)(SO_4)_2 + 1 M HClO_4$)
- 11. 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.

Essential/recommended readings

Theory:

- 1. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 2A: Fundamentals of Electrodics 2nd Ed., Springer (2001).
- 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. Bard, A. J. Faulkner, L. R. Electrochemical Methods: Fundamentals and Applications, 2nd Ed., John Wiley & Sons: New York, 2002.
- 4. Oldham, K. B., Myland, J. C. and Bond, A. M. Electrochemical Science and Technology: Fundamental and Applications, John Wiley & Sons, Ltd. (2012).
- 5. Brett, C. M. A. & Brett, A. M. O. Electrochemistry, Oxford University Press (1993).
- 6. Koryta, J., Dvorak, J. & Kavan, L. Principles of Electrochemistry John Wiley & Sons: NY (1993).
- 7. Bagotsky, V.S., Fundamentals of Electrochemistry 2nd Ed. Wiley Interscience, (2006)
- 8. Hamann, Carl H., Hamneff, Andrew & Vielstich, Wolf., Electrochemistry, 2nd Ed. (2007)

Practical:

- 1. Khosla B. D., Garg V. C., Gulati A., Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
- 2. Holze R., (2019) Experimental Electrochemistry: A laboratory Textbook, Wiley-VCH.
- 3. Brabec V., Walz D., Milazzo G., Experimental techniques in Bioelectrochemistry, Springer.
- 4. Bartlett P. N., Bioelectrochemistry: Fundamentals, Experimental Techniques and Applications, John Wiley & Sons Inc.
- 5. 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.
- 6. Field, R. J.; Schneider, F. W. Oscillating Chemical Reactions and Nonlinear Dynamics, *J. Chem. Educ.* **1989**, *66*, *3*, 195–204.
- 7. King D, Friend J., Kariuki J., Measuring Vitamin C Content of Commercial Orange Juice Using a Pencil Lead Electrode, J. Chem. Educ. **2010**, 87, 5, 507–509.
- 8. Lima D, Singh V, Bulleeraz K, Lussier J. A., Kuss S., Electrifying Fruit Juice: Integrating Applied Electroanalytical Chemistry into the Undergraduate Curriculum, *J. Chem. Educ.* **2024**, *101*, *7*, *2938-2946*.

DISCIPLINE SPECIFIC ELECTIVE COURSE – 24 LS (DSE-24 LS)

Nanomaterials and their Biological Applications

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title &	Credits	Credit distribution of the course			Eligibility	Pre-requisite
Code		Lecture	Tutorial	Practical/	criteria	of the course
				Practice		(if any)
Nanomaterials	04	02		02	Class12 th	
and their					with	
Biological					Physics,	
Applications					Chemistry	
(DSE-24 LS)					Biology	

Course Objectives

The objectives of this course are as follows:

- To study about fundamentals and applications of Advanced Inorganic materials.
- To understand the mechanism of synthesis of hydrogels, composites, mesoporous materials.
- To understand the fabrication of materials for their notable applications in living systems.
- To know how these materials are making life easier in this era and are great sources of industrial growth and technological changes.

Learning outcomes

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

- Understand various materials, their synthesis and properties.
- Explain the mechanism of growth of self-assembled nanostructures.
- Explain the importance of hydrogels composites, mesoporous materials and their applications.
- Understand the usage of materials in various fields ranging from modern life to Human health, and environment.
- Develop skills in the scientific method of planning, developing, conducting, reviewing and reporting experiments.

Unit1: Nanomaterials (8 Hours)

Overview of nanostructures and nanomaterials, classification, preparation and optical properties of gold and silver metallic nanoparticles, concept of surface plasmon resonance, carbon nanotubes, inorganic nanowires, Bioinorganic nanomaterials, DNA and its nanomaterials, natural and artificial nanomaterials, self-assembled nanostructures, control of nanoarchitecture, one dimensional control.

Unit 2: Composite materials

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.

(7 Hours)

Unit 3: Hydrogels: (10 Hours)

Introduction, natural, synthetic, and hybrid hydrogels, Properties of hydrogels, different methods of synthesis, notable hydrogel systems such as alginate-based, PEGDA, and PVA hydrogels, Applications of hydrogels such as environmental remediation, Food packaging, sensor, and biomedical.

Unit 4: Nanomaterials for Biomedical Applications

(5 Hours)

Inorganic nanomaterials: silica, carbon based, metallic, oxides.

Biomedical applications: Quantum dots, gold nanoparticles, and magnetic nanoparticles for imaging, biosensing, therapeutics and diagnostics. Polymeric nanoparticles, dendrimers, and carbon nanotubes applied to drug delivery systems. Nanomaterials such as nanofibers, and nanocomposite materials as scaffold materials for tissue engineering and regeneration. Nanotoxicology.

Practical: Credits: 02

- 1. Synthesis of hydrogels and study of swelling behavior.
- 2. Preparation of zeolite A and removal of Mg and Ca ions from water samples quantitatively using zeolite.
- 3. Synthesis of ZnO, NiO nanoparticles by green approach methods and characterization using UV-visible spectrophotometer.
- 4. Synthesis of Cu doped ZnO nanoparticles.
- 5. Synthesis of CuS, MnS and CdS nanoparticles and their characterization using UV- visible spectrophotometer.
- 6. Synthesis of gold and silver nanoparticles and study of their optical properties as a function of size.

Recommended Texts:

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. Xu, C.; Zang Y. S.; Begin S.; Thanh N. T. K.; Nanoscale, 2022,14, 7441-7443.
- 5. Poole Jr.; Charles P.; Owens, Frank J. (2003), Introduction to Nanotechnology, John Wiley and Sons.

Practical:

- 1. Cheng, K.H.; Jacobson, A.J.; Whittingham, M.S. (1981), Hexagonal Tungsten Trioxide and Its Intercalation Chemistry, Solid State Ionics, 5, 1981, 355-358.
- 2. Ghorbani H.R.; Mehr, F.P; Pazoki, H; Rahmani, B.M.; Synthesis of ZnO Nanoparticles by Precipitation Method, Orient J Chem 2015, 31(2).
- 3. A.K. Sharma, R. Sharma, B. Pani, A. Sarkar, M. Tripathi, Engineering the Future with Hydrogels: Advancements in Energy Storage Devices and Biomedical Technologies. New Journal of Chemistry, RSC, 2024, 48, 10347-10369.
- 4. Xu, C.; Zang Y. S.; Begin S.; Thanh N. T. K.; Nanoscale, 2022,14, 7441-7443.

<u>List of Instruments/Software required for Implementation of Fourth year Course of Study for each College</u>

- 1. UV- Vis Spectrophotometer
- 2. Table top IR Spectrophotometer
- 3. ChemDraw, GaussView6/ GaussView5 and Gaussian 16/Gaussian 09 Software
- 4. Access to p-XRD NMR Spectrophotometer in Department of Chemistry/USIC
- 5. Rota Evaporator
- 6. Sonicator
- 7. Cyclic Voltammeter/ Potentiostate-Galvanostate