ANNEXURE-4.02.03
AC-26.05.2023

DEPARTMENT OF CHEMISTRY
SEMESTER-IV

SL.NO.	SUBJECT	PAGE NO.
1	**SEMESTER-IV** **BSc. (Hons.) Chemistry - DSC** 1. Coordination Chemistry and Reaction Mechanism 2. Carbohydrates, Lipids and Hetero cyclic Compounds 3. Electrochemical Cells, Chemical Kinetics and Catalysis **Pool of DSE for III/IV/V/VI Semester** 1. Inorganic Materials of Industrial Importance 2. Green Chemistry in Organic Synthesis 3. Solutions, Colligative properties, Phase Equilibria and adsorption 4. Nuclear and Environmental Chemistry 5. Reactions, Reagents and Chemical Process 6. Polymers, Colloids, Surfaces and Interfaces 7. Novel Inorganic Solids 8. Applied Organic Chemistry 9. Applications of Computers in Chemistry 10. Analytical Methods in Chemistry 11. Basic Principles of Food Chemistry 12. Computational Methods & Molecular Modelling **13.** Research Methodology for Chemists	2-63
2	**SEMESTER-V** **BSc. (Hons.) Chemistry – DSC** 1. Basics of Organometallic Chemistry 2. Nucleic Acids, Amino Acids, Proteins and Enzymes 3. Quantum Chemistry and Covalent bonding	55-64

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

DISCIPLINE SPECIFIC ELECTIVE COURSE - 1 (DSE-1): Inorganic Materials of Industrial Importance

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Inorganic Materials of Industrial Importance (DSE-1)	**04**	**03**	**--**	**01**	Class 12th with Physics, Chemistry	--

Learning Objectives

The objectives of this course are as follows:

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

Learning outcomes

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

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

SYLLABUS OF DSE-1

Unit 1: Silicate Industries **(2 Weeks)**

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, different types of safety glass, borosilicate glass, fluorosilicate glass, coloured glass, photosensitive glass, photochromic glass, glass wool and optical fibre.

Cement: Manufacture of Portland cement and the setting process, Different types of cements: quick setting cements, eco-friendly cement (slag cement), pozzolana cement.

Unit 2: Fertilizers (2 Weeks)

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

Unit 3: Surface Coatings (6 Weeks)

Brief introduction to and classification of surface coatings, paints and pigments: formulation, composition and related properties, pigment volume concentration (PVC)and critical pigment volume concentration (CPVC), fillers, thinners, enamels and emulsifying agents. Special paints: heat retardant, fire retardant, eco-friendly paints, plastic paints, water and oil paints. Preliminary methods for surface preparation, metallic coatings (electrolytic and electroless with reference to chrome plating and nickel plating), metal spraying and anodizing.

Contemporary surface coating methods like physical vapor deposition, chemical vapor deposition, galvanising, carburizing, sherardising, boriding, nitriding and cementation.

Unit 4: Batteries (3 Weeks)

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

Unit 5: Nano dimensional materials (2 Weeks)

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

Practical component

Practicals: Credits:

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

(At least four experiments to be performed)

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

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

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

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

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

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

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

Essential/recommended readings

Theory:

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

Practical:

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

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

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

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Green Chemistry in Organic Synthesis (DSE-2)	04	03	--	01	Class 12^{th} with Physics, Chemistry	Basic knowledge of organic reactions

Learning objectives

The objectives of this course are as follows:

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

Learning outcomes

By studying this course, students will be able to:

- List the twelve principles of green chemistry and build the basic understanding of toxicity, hazard and risk related to chemical substances.
- Calculate atom economy, E-factor and relate them in all organic synthesis
- State the uses of catalyst over stoichiometric reagents

- Debate and use green solvents, renewable feedstock, and renewable energy sources for carrying out safer chemistry
- Use green chemistry for problem solving, innovation and finding solutions to environmental problems.
- Design safer processes, chemicals, and products through understanding of inherently safer design (ISD)
- Discuss the success stories and use real-world cases to practice green chemistry

SYLLABUS OF DSE-2

UNIT – 1: Introduction **(1 Week)**

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

UNIT – 2: **Application of Green Chemistry Principles** **(12 Weeks)**

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

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

v. Visible light induced Reactions: with examples such as, syntheses of caprolactam and vitamin D_3, cis-trans isomerization of alkenes

6. Use of renewable starting materials: Illustrate with few examples such as biodiesel, bioethanol, polymers from renewable resources (PLA from corn), Synthesis and properties of 2-Methyltetrahydrofuran, furfural and 5-Aminolevulinic acid (DALA) from levulinic acid
7. Avoidance of unnecessary derivatization – careful use of blocking/protecting groups (taking specific examples like selective oxidation of aldehydic group and synthesis of 6-Aminopenicillanic Acid (6-APA) from penicillin G
8. Catalysis and green chemistry
   Introduction to Catalysis (including concept of selectivity, turnover frequency and turnover number), Types of Catalysts: Heterogeneous catalysis and homogeneous catalysis (H-beta and zeolites in organic synthesis), General catalytic cycle for heterogeneous catalysis; Asymmetric catalysis (Monsanto route to L-dopa via asymmetric hydrogenation, synthesis of carbapenhem via Asymmetric reduction); Photocatalysis (with special reference to TiO2); Biocatalysis (Synthesis of adipic acid/catechol using biocatalyst) and Nanocatalysis (oxazole synthesis using nanocatalyst)
9. Design for degradation: (Illustrate with the help of examples: soaps and detergents, pesticides, polymers)
10. Real Time monitoring of chemical processes using inline, offline, and online techniques
11. Inherently safer design/chemistry:
    Principle and subdivision of ISD, Bhopal Gas Tragedy (safer route to carbaryl) and Flixiborough accident (safer route to cyclohexanol, Asahi Process)

UNIT – 3: Industrial Applications and Success Stories (2 Weeks)

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

Practical component Credits:

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

Note: Characterization by melting point, UV-Visible spectroscopy, IR spectroscopy and any other specific method should be done (wherever applicable).

1. Preparation and characterization of nanoparticles of gold using tea leaves/silver nanoparticles using plant extracts.
2. Preparation of biodiesel from waste cooking oil and characterization (TLC, pH, solubility, combustion test, density, viscosity, gel formation at low temperature and IR can be provided).
3. Benzoin condensation using thiamine hydrochloride as a catalyst instead of cyanide.
4. Extraction of D-limonene from orange peel using liquid CO2 prepared from dry ice.

5. Mechanochemical solvent free, solid-solid synthesis of azomethine using p-toluidine and o-vanillin/p-vanillin.
6. Microwave-assisted Knoevenagel reaction using anisaldehyde, ethylcyanoacetate and ammonium formate.
7. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
8. Photochemical conversion of dimethyl maleate to dimethyl fumarate (cis-trans isomerisation)
9. Benzil- Benzilic acid rearrangement: Preparation of benzilic acid in solid state under solvent-free condition.
10. Preparation of dibenzalacetone by cross aldol condensation reaction using base catalysed green method.

Essential/recommended readings

Theory:

1. Anastas, P.T., Warner, J.C. (2014), **Green Chemistry, Theory and Practice**, Oxford University Press.
2. Lancaster, M. (2016), **Green Chemistry: An Introductory Text**, 3rd Edition, RSC Publishing.
3. Cann, M. C., Connely, M.E. (2000), **Real-World cases in Green Chemistry, American Chemical Society**, Washington.
4. Matlack, A.S. (2010), **Introduction to Green Chemistry**, 2nd Edition, Boca Raton: CRC Press/Taylor & Francis Group publisher.
5. Alhuwalia,V.K., Kidwai, M.R. (2005), **New Trends in Green chemistry**, Anamalaya Publishers.
6. Sidhwani, I.T, Sharma, R.K. (2020), **An Introductory Text on Green Chemistry**, Wiley India Pvt Ltd.

Practicals:

1. Kirchoff, M.; Ryan, M.A. (2002), **Greener approaches to undergraduate chemistry experiment**, American Chemical Society, Washington DC.
2. Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K. (2013), **Green Chemistry Experiments: A monograph**, I.K. International Publishing House Pvt Ltd. New Delhi.
3. Pavia, D.L.; Lamponam, G.H.; Kriz, G.S.W. B. (2012), **Introduction to organic Laboratory Technique- A Microscale approach**, 4th Edition, Brooks-Cole Laboratory Series for Organic chemistry.
4. Sidhwani I.T. (2015), Wealth from Waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated. **DU Journal of Undergraduate Research and Innovation**, 1(1),131-151. ISSN: 2395-2334.
5. Sidhwani, I.T; Sharma, R.K. (2020), **An Introductory Text on Green Chemistry**, Wiley India Pvt Ltd.
6. **Monograph on Green Chemistry Laboratory Experiments**, Green Chemistry Task Force Committee, Department of Science and Technology, Government of India.
7. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi
8. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi

DISCIPLINE SPECIFIC ELECTIVE COURSE -3(DSE-3): Solutions, Colligative properties, Phase Equilibria and adsorption

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Solutions, Colligative properties, Phase Equilibria and adsorption (DSE-3)	**04**	**03**	**-**	**01**	Class 12th with Physics, Chemistry	

Learning Objectives

The Learning Objectives of this course are as follows:

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

Learning outcomes

By studying this course, students will be able to:

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

SYLLABUS OF DSE-3

UNIT-1: Solutions and Colligative Properties **(4 Weeks)**

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

UNIT-2: Phase Equilibria (8 Weeks)

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

UNIT-3: Surface chemistry (3 Weeks)

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

Practical component Credit: 01

(Laboratory periods: 15 classes of 2 hours each)

Practical

Phase Equilibrium

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

Adsorption

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

Essential/recommended readings

Theory:

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

Practical:

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

Suggestive readings

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

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

DISCIPLINE SPECIFIC ELECTIVE COURSE -4 (DSE-4): Nuclear and Environmental Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Nuclear and Environmental Chemistry (DSE-4)	**04**	**03**	**--**	**01**	Class 12th with Physics, Chemistry	**--**

Learning Objectives

The Objectives of this course are as follows:

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

Learning outcomes

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

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

SYLLABUS OF DSE-4

Unit-1 : Nuclear Chemistry **(7 Weeks)**

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

UNIT – 2: Air Pollution (4 Weeks)

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

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

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

UNIT – 3 : Water Pollution: (4 Weeks)

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

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

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

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

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

Essential/recommended readings

Theory:

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

Practical:

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

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

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

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Reactions, Reagents and Chemical Process (DSE-5)	04	03	--	01	Class 12th with Physics, Chemistry	Basic knowledge of organic reactions

Learning objectives

The objectives of this course are as follows:

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

Learning outcomes

By studying this course, students will be able to:

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

SYLLABUS OF DSE-5

UNIT – 1: Name Reactions **(5 Weeks)**

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

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

UNIT – 2: **Reducing Reagents** **(3 Weeks)**

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

UNIT – 3: Oxidizing Reagents **(3 Weeks)**

Reactions, mechanism and applications of following oxidizing agents: Jones Reagent (CrO_3, H_2SO_4, H_2O), Swern Reagent (DMSO, oxalyl chloride), Dess Martin, TEMPO, TPAP (Tetrapropyl ammonium perruthenate), Fetizon's Reagent, Fenton's Reagent [H_2O_2 + Fe(II) ion], Sodium perborate NaH_2BO_4, Sodium Bismuthate $NaBiO_3$, ABNO (9-Azabicyclo[3.3.1]nonane N-oxyl), DEAP (Diethyl allyl phosphate, ), AZADO (2-Azaadamantane N-oxyl], Wacker oxidation.

UNIT – 4: Process Chemistry **(4 Weeks)**

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

Practical component **Credits:**

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

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

Essential/recommended readings

Theory:

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

Practical:

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

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

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

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Polymers, Colloids, Surfaces and Interfaces (DSE- 6)	**04**	**03**	**--**	**01**	Class 12th with Physics, Chemistry	**--**

Learning Objectives

The objectives of this course are as follows:

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

Learning outcomes

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

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

SYLLABUS OF DSE-6

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

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

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

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

UNIT 3: Introduction to Colloid Chemistry (Lectures: 9)

Recapitulation of basic concepts of Adsorption, Distinction among true solutions, colloids and suspensions, Components of Colloids, classification of colloids - lyophilic, lyophobic; Preparation methods and properties of lyophobic solutions, Hydrophile-lyophile balance (HLB), multi molecular, macromolecular and associated colloids (micelles formation), preparation and properties of colloids - Tyndall effect, Brownian movement, electrophoresis, dialysis, coagulation and flocculation; Charge on Colloidal particles and Electrical double layer concept, Suspensions and their characteristics, Emulsions and their characteristics.

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

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

UNIT 5: Application of colloids (Lectures: 9)

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

Practical component

Practicals: Credits: 01

(Laboratory periods:15 classes of 2 hours each)

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

B. Antimony sulphide

C. Ferric chloride

D. Aluminium hydroxide

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

Essential/recommended readings

Theory:

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

Practical:

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

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

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

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Novel Inorganic Solids (DSE-7)	**04**	**03**	**--**	**01**	**Class 12th with Physics, Chemistry**	**--**

Learning Objectives

The Objectives of this course are as follows:

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

Learning Outcomes:

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

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

SYLLABUS OF DSE- 7

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

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

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

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

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

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

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

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

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

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

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

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

Practicals **Credits: 01**

(Laboratory periods: 15 classes of 2 hours each)

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

   (i) $PbCrO_4$ / chrome yellow

   (ii) Barium white

   (iii) Prussian Blue

   (iv) Malachite

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

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

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

Essential/recommended readings

Theory:

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

Practicals:

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

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

DISCIPLINE SPECIFIC ELECTIVE COURSE – 8 (DSE-8): Applied Organic Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Applied Organic Chemistry (DSE-8)	04	03	--	01	Class 12th with Physics, Chemistry	--

Learning Objectives

The objectives of this course are as follows:

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

Learning outcomes

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

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

SYLLABUS OF DSE-8

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

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

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

Unit 2: Polymers **(Lectures:12)**

Introduction and classification based on origin, monomer units, thermal response, mode of formation, structure, application and tacticity; di-block, tri-block and amphiphilic polymers; Weight average molecular weight, number average molecular weight, glass transition temperature (Tg) of polymers; Polymerisation Reactions-Addition and condensation. Mechanism of cationic, anionic and free radical addition polymerization; Ziegler-Natta polymerisation of alkenes.

Preparation and applications of: Plastics -thermosetting (phenol-formaldehyde, Polyurethanes) and thermosoftening (PVC, polythene); Fabrics -natural (cellulose and synthetic derivatives of cellulose like rayon and viscose); synthetic (acrylic, polyamide, polyester); Rubbers-natural and synthetic: Buna-N, Buna-S, Neoprene, silicon rubber; Vulcanization; Polymer additives; Introduction to Specialty Polymers: electroluminescent (Organic light emitting diodes), Conducting, biodegradable polymers and liquid crystals.

Unit 3: Natural Product Chemistry- An Introduction to Terpenoids, Alkaloids and Steroids (Lectures: 12)

Terpenes: Introduction, occurrence, classification, uses, isoprene and special isoprene rule; structure elucidation, synthesis and industrial application of citral.

Alkaloids: Introduction, occurrence, classification, uses, general structural features, general methods for structure elucidation including Hoffmann's exhaustive methylation and Emde's method. Structure elucidation, synthesis and physiological action of Nicotine.

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

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

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

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

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

Practical component

Practical: **Credits: 01**

(Laboratory periods:15 classes of 2 hours each)

(At least five experiments to be performed)

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

Essential/recommended readings

Theory:

1. Finar, I.L. Fifth Edition **Organic Chemistry**, Volume 2, Pearson Education, 2008.
2. Saunders, K. J., (1988), **Organic Polymer Chemistry,** Second Edition Chapman & Hall, London.
3. Campbell, Ian M., (2000), **Introduction to Synthetic Polymers**, Second Edition, Oxford University Press, USA.
4. Bahadur, P. and Sastry, N.V. (2002) **Principles of Polymer Science** Narosa, New Delhi
5. Patrick, G. **An Introduction to Medicinal Chemistry** (2013), Fourth Edition, Oxford University Press.
6. Beale J.M. Block J., (2010) **Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry,** Twelfth Edition, Lippincott Williams and Wilkins.
7. Alagarsamy, V. (2010), **Textbook of Medicinal Chemistry**, Volume II, Second Edition, Reed Elsevier India Private Limited.

Practical:

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

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

DISCIPLINE SPECIFIC ELECTIVE COURSE- 9 (DSE-9): Applications of Computers in Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Applications of Computers in Chemistry (DSE 9)	**04**	**03**	**-**	**01**	Class 12th with Physics, Chemistry	

Learning Objectives

The Objectives of this course are as follows:

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

Learning outcomes

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

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

SYLLABUS OF DSE-9

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

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

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

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

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

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

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

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

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

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

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

Practical component

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

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

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

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

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

Essential/recommended readings

Theory:

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

Practical

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

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

DISCIPLINE SPECIFIC ELECTIVE COURSE - 10(DSE-10): Analytical Methods in Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Analytical Methods in Chemistry (DSE-10)	**04**	**03**	**--**	**01**	**Class 12th with Physics, Chemistry**	**-**

Learning Objectives

The Objectives of this course are as follows:

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

Learning Outcomes:

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

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

SYLLABUS OF DSE-10

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

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

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

Unit 2: Optical Methods of Analysis (Lectures: 25)

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

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

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

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

Unit 3: Thermal methods of analysis (Lectures: 5)

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

Unit 4: Separation techniques (Lectures:10)

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

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

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

Practicals Credits 01

(Laboratory periods: 15 classes of 2 hours each)

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

2. Solvent Extractions

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

3. Analysis of soil:

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

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

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

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

Essential/recommended readings

Theory:

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

Practicals:

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

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

DISCIPLINE SPECIFIC ELECTIVE COURSE - 11 (DSE-11): Basic Principles of Food Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Basic Principles of Food Chemistry (DSE-11)	04	03	--	01	Class 12th with Physics, Chemistry	--

Learning Objectives

The objectives of this course are as follows:

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

Learning outcomes

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

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

SYLLABUS OF DSE-11

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

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

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

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

Unit 3: Carbohydrates (Lectures:6)

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

Unit 4: Proteins (Lectures:6)

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

Unit 5: Lipids (Lectures:6)

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

Unit 6: Vitamins and Minerals (Lectures:6)

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

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

Unit 7: Food Additives (Lectures:15)

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

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

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

Practical component

Practical: **Credits: 01**

(Laboratory periods:15 classes of 2 hours each)

(At least four experiments to be performed)

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

Essential/recommended readings

Theory:

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

Practical:

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

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

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

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Computational Methods & Molecular Modelling (DSE-12)	**04**	**03**	**--**	**01**	Class 12th with Physics, Chemistry and Mathematics	**--**

Learning Objectives

The Objectives of this course are as follows:

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

Learning outcomes

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

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

SYLLABUS OF DSE-12

UNIT-1 : Introduction **(Lectures: 6)**

Introduction to computational chemistry: Overview of Classical and Quantum Mechanical Methods (Ab initio, DFT, Semi-empirical, Molecular Mechanics, Molecular Dynamics, and Monte Carlo)

UNIT – 2: Potential Energy Surfaces **(Lectures: 6)**

Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global minima, Geometry optimization and energy minimization, the concept of transition state with examples, Hessian matrix

UNIT – 3 : Molecular Mechanics & Molecular Dynamics **(Lectures: 9)**

Molecular Mechanics

Force Fields (A brief explanation of all the terms of a basic force field), the basic idea of MM1, MM2, MM3, MM4, MM+, AMBER, BIO+, OPLS.

Molecular Dynamics

The concept of the periodic box, ensembles (microcanonical, canonical, isothermal – isobaric), steps in a typical MD simulation.

UNIT-4: Huckel Molecular Orbital Theory **(Lectures: 6)**

Huckel MO with examples: ethene and propenyl systems, Properties calculated – energy, charges, bond order, electronic energies, resonance energies.

UNIT- 5: Computational Methods **(Lectures: 18)**

Ab-initio methods

Antisymmetry principle, Slater determinants, SCF method, Hartree-Fock method.
Basis sets, Basis functions, STOs and GTOs, diffuse and polarization functions. Minimal basis sets, Basis set superposition error (BSSE) - Effective core potentials (ECP)
Advantages of ab initio calculations.

Density Functional Theory

A brief description of Density Functional Theory (DFT). Calculation of Electronic Properties in ground and Excited states

Semi-empirical methods

Basic idea about Zero differential overlap (ZDO) approximation

Some important concepts

Concepts of atomic charges, electrostatic potential maps, computation of thermodynamic properties and spectroscopic observables

Practical component

Practical: Credits: 01

(Laboratory periods:15 classes of 2 hours each)

1) Write the Z-Matrix of a given set of molecules.

2) Carry out geometry optimisation on H_2O, H_2S, H_2Se molecules compare the optimized bond angles and dipole moments from the results obtained. Obtain the ESP-mapped density surfaces and interpret the results obtained with reference to bonding in these molecules.

   Suggestive: A comparative analysis of results of the above exercise may be carried out using different quantum mechanical methods.

3) Calculate the energy of the following chemical species and arrange them in order of increasing stability.

   1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3- dimethyl-2-butene in order of increasing stability.

4) Carry out geometry optimisation on the following chemical species and compare the shapes and dipole moments of the molecules.

   1-pentanol, 2-pentanol, 3-pentanol, 2-methylbutan-1-ol, 3-methylbutan-1-ol, 2-methylbutan-2-ol, 2-methylbutan-3-ol and 2,2-dimethylpropanol.

   Correlate the computationally obtained values of the dipole moments with the experimental values of the boiling points: (118 ºC, 100 ºC, 108 ºC, 82 ºC, of 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2- propanol respectively).

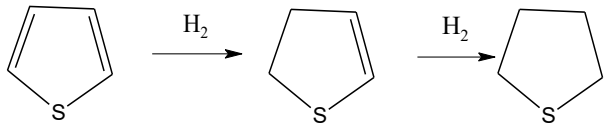
5) Based on the implicit electronic structure calculations, determine the heat of hydrogenation of Propylene.

6) Based on the calculations of enthanlies of the participating chemical species on optimized geometry of the molecules, calculate the reaction enthalpy at 298 K for the following, industrially important reactions:

   $$CH_4 + H_2O \rightarrow CO + 3H_2$$ (steam reforming of methane)

   ≡≡ (Haber-Bosch process)

7) Carry out geometry optimisation and determine the energy of the participating chemical species in the following reactions Using these results calculate the resonance energy of thiophene.



8) Carry out geometry optimisation & Energy calculations on the following species and obtain Frontier Molecular Orbitals. Visualize the Molecular Orbitals of these species and interpret the results for bonding in these molecules.
Benzene, Naphthalene, and Anthracene.

9) Compare the gas phase basicities of the methylamines by comparing the enthalpies of the following reactions:

$$BH^+ + NH_3 \rightarrow B + NH_4^+$$

Where B = CH_3NH_2, $(CH_3)_2NH$, $(CH_3)_3N$

10) On the basis of results of geometry optimization and energy calculations, determine the enthalpy of isomerization of cis and trans 2-butene.

11) Perform a conformational analysis of butane. Plot the graph between the angle of rotation and the energy of the conformers using spreadsheet software.

12) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.

13) Calculate the electronic UV/Visible absorption spectrum of Benzene.

14) Calculate the electronic absorption spectra of formaldehyde.

15) Plot the electrostatic potential mapped on electron density for benzene and use it to predict the type of stacking in the crystal structure of benzene dimer.

16) On a given set of molecules methylamine (CH_3NH_2) carry out geometry optimization, single point energy and NBO calculations and interpret the output results treated at the ab initio RHF/3-21G level.

17) Study the mechanism of SN_2 reaction between Cl^- and CH_3Br involving a Walden inversion computationally.

18) Perform a geometry optimization followed by a frequency assessment (opt+freq keyword) using the B3LYP method and 6-31-G(d) basis set on a given set of small molecules i.e. BH_3, CH_4.
Suggestive: A greater number of molecules may be studied as per instructions received from the concerned teacher.

19) Based on the fundamentals of conceptual DFT calculate the ionization potential (IP), electron affinity (EA), electronegativity and electron chemical potential of a given set of molecules.

20) Perform molecular docking of Sulfonamide-type D-Glucose inhibitor into MurrD active site using Argus Lab.

21) Perform molecular dynamics (MD) simulation of a given alkali metal ion in aqueous function (RDF)

Essential/recommended readings

Theory:

1. Lewars, E. (2003), **Computational Chemistry**, Kluwer academic Publisher.
2. Cramer, C.J. (2004), **Essentials of Computational Chemistry**, John Wiley & Sons.
3. Hinchcliffe, A. (1996), **Modelling Molecular Structures**, John Wiley & Sons.
4. Leach, A.R. (2001), **Molecular Modelling**, Prentice-Hall.
5. House, J.E. (2004), **Fundamentals of Quantum Chemistry**, 2nd Edition, Elsevier.
6. McQuarrie, D.A. (2016), **Quantum Chemistry**, Viva Books.
7. Levine, I. N.; **Physical Chemistry**, 5th Edition, McGraw –Hill.

Practical:

1. https://www.afs.enea.it/software/orca/orca_manual_4_2_1.pdf
2. https://dasher.wustl.edu/chem430/software/avogadro/learning-avogadro.pdf
3. http://www.arguslab.com/arguslab.com/ArgusLab.html
4. https://barrett-group.mcgill.ca/tutorials/Gaussian%20tutorial.pdf
5. https://gaussian.com/techsupport/
6. https://gaussian.com/man/
7. https://gaussian.com/wp-content/uploads/dl/gv6.pdf
8. https://dasher.wustl.edu/chem478/software/spartan-manual.pdf
9. http://www.mdtutorials.com/gmx/
10. https://vina.scripps.edu/manual/

Important Instruction Note on working approach:

- A student is required to perform/investigate a minimum of 10 exercises from the given set of exercises.
- The students may use open source softwares; ArgusLab, Avogadro and ORCA. In case a licenced version softwares is available, if procured by the college, other licenced softwares may also be used.

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

DISCIPLINE SPECIFIC ELECTIVE COURSE – 13 (DSE-13): Research Methodology for Chemists

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Research Methodology for Chemists (DSE-13)	04	03	--	01	Class 12th with Physics, Chemistry	

Learning objectives

The objectives of this course are as follows:

- To make the students aware of fundamental but mandatory ethical practices in chemistry.
- To introduce the concept of data analysis.
- To learn to perform literature survey in different modes.
- To make the students aware of safety handling and safe storage of chemicals.
- To make students aware about plagiarism and how to avoid it.
- To teach the use of different e-resources.

Learning outcomes

By studying this course, students will be able to:

- Follow ethical practices in chemistry
- Do Data analysis
- Literature survey in different modes
- Use e-resources.
- Avoid plagiarism, understand the consequences and how to avoid

SYLLABUS OF DSE-13

UNIT – 1: Scope of Research **(Lectures: 3)**

Introduction, overview of research process: define research problem, review literature, formulate hypothesis, design research/experiment, collect and analyse data, interpret and report, scope and importance.

UNIT – 2: **Literature Survey, Databases and Research metrics** **(Lectures: 15)**

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, Digital: Databases and their responsible use: Google Scholar, Web of science, Scopus, UGC INFONET, SciFinder, PubMed, ResearchGate, E-consortium, e-books; Search techniques: Phrase, Field, Boolean, Proximity, Concept, Limiting/Refining Search Results.
Research metrics: Impact factor of Journal, h-index, i10 index, Altmetrics, Citation index.
Author identifiers/or profiles: ORCID, Publons, Google Scholar, ResearchGate, VIDWAN

UNIT – 3: Communication in Science **(Lectures: 12)**

Types of technical documents: Full length research paper, book chapters, reviews, short communication, project proposal, Letters to editor, and thesis.
Thesis writing – different steps and software tools (Word processing, LaTeX, Chemdraw, Chemsketch etc) in the design and preparation of thesis, layout, structure (chapter plan) and language of typical reports, Illustrations and tables, bibliography, referencing: Styles (APA, Oxford etc), annotated bibliography, Citation management tools: Mendeley, Zotero and Endnote; footnotes. Oral presentation/posters – planning, software tools, creating and making effective presentation, use of visual aids, importance of effective communication, electronic manuscript submission, effective oral scientific communication and presentation skills.

UNIT – 4: Research and Publication ethics **(Lectures: 9)**

Scientific Conduct: Ethics with respect to science and research, Scientific Misconducts: falsification, fabrication and plagiarism, similarity index, software tools for finding plagiarism (Turnitin, Urkund etc), redundant dublications

Publication Ethics: Introduction, COPE (Committee on Publication Ethics) guidelines; conflicts of interest, publication misconduct: problems that lead to unethical behaviour and vice versa, types, violation of publication ethics, authorship and contributorship, predatory publishers and journals

IPR - Intellectual property rights and patent law, commercialization, copy right, royalty, trade related aspects of intellectual property rights (TRIPS)

UNIT – 5: Statistical analysis for chemists **(Lectures: 6)**

Types of data, data collection-Methods and tools, data processing, hypothesis testing, Normal and Binomial distribution, tests of significance: t-test, F-test, chi- square test, ANOVA, multiple range test, regression and correlation.

Features of data analysis with computers and softwares -Microsoft Excel, Origin, SPSS

Practical component **Credits: 01**

(Laboratory periods:15 classes of 2 hours each)

1. Collection of journal articles on a particular topic using Google Scholar and creating a database.
2. Collection of journal articles on a particular topic using Science Direct and creating a database.
3. Collection of journal articles on a particular topic using Scopus and creating a database.
4. Drawing chemical structure, reactions and mechanisms using Chemsketch or ISIS draw or any other software.
5. Collection of chemical structure using ChemSpider and creating a database.
6. Curve fitting using freely available softwares/apps (any one)
7. Making of power point presentation
8. Experimental learning of safe storage hazardous chemicals
9. Experimental learning of handling of hazardous chemicals
10. Technical writing on topics assigned.
11. Demonstration for checking of plagiarism using recommended software

Essential/recommended readings:

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) Practical skills in chemistry. 2nd Ed. Prentice-Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) Data analysis for chemistry. Oxford University Press.
3. Topping, J. (1984) Errors of observation and their treatment. Fourth Ed., Chapman Hall, London.
4. Harris, D. C. Quantitative chemical analysis. 6th Ed., Freeman (2007) Chapters 3-5.
5. Levie, R. de, how to use Excel in analytical chemistry and in general scientific data analysis. Cambridge Univ. Press (2001) 487 pages.
6. Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
   OSU safety manual 1.01

Note:

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

- **The students are required to opt one paper each from DSEs 1-3 in Semester 3, DSEs 4-6 in Semester 4, DSEs 7-9 in Semester 5 and DSEs 10-13 in Semester 6.**

- **Research Methodology (DSE 13) shall be offered as one of the DSE courses in semester VI or VII. If a student wishes to pursue four years Honours Degree with Research, he/she shall compulsorily opt for a Research Methodology course in either Semester VI or VII.**