INDEX

DEPARTMENT OF CHEMISTRY

SEMESTER – II

B.Sc. (Hons.) with Analytical Chemistry

Analytical Chemistry

COURSES OFFERED BY THE DEPARTMENT OF CHEMISTRY

Category II

B.Sc. in Analytical Chemistry Course for Undergraduate Programme of study with Analytical Chemistry as one of the Core Discipline

(B.Sc. H with Analytical Chemistry)

Semester	Core (DSC) 4 credits	Elective (DSE) 4 credits	Generic Elective (GE) 4 credits	Ability Enhance-ment Course (AEC) – 2 credits	Skill Enhance-ment Course (SEC) – 2 credits	Internship/ Apprentice-ship/Project/ Community outreach 2 credits	Value addition course (VAC) 2 credits	Total Credits
II	DSC - 4 DSC - 5 DSC - 6	NIL	Choose one from a pool of courses GE-2 (4)	Choose one from a pool of AEC courses (2)	Choose one from a pool of SEC courses (2)	NIL	Choose one from a pool of VAC courses (2)	22 credits

STRUCTURE OF SECOND SEMESTER

A student who pursues undergraduate programme with Analytical Chemistry as multidisciplinary core discipline is offered the following courses:

3 Discipline Specific Cores (DSCs) - 3 courses of 4 credits = 12 credits (Two DSCs are offered by the parent Department of Chemistry and one DSC is offered by the Department of Mathematics).

0 Discipline Specific Electives (DSE) – No DSE courses in Semester I (offered by the parent Department i.e. Department of Chemistry as choice based electives

1 Generic Elective (GE) – 1 course of 4 credits = 4 credits: one course to be chosen from the common pool of GE courses offered by Departments other than the parent Department(s).

1 Ability Enhancement Course (AEC) – 1 course of 4 credits = 4 credits (one course to be chosen from either 'Environmental Science: Theory to Practice' or one of the 22 Indian Languages listed in the 8^{th} Schedule of the Constitution in the pool of AEC courses)

1 Skill Enhancement Course (SEC) - 1 course of 4 credits = 4 credits (one course to be chosen from the common pool of SEC courses offered by any Department)

1 Value Addition Course (VAC) - 1 course of 4 credits = 4 credits (one course to be chosen from the common pool of VAC courses offered by any Department)

DISCIPLINE SPECIFIC CORE COURSE – 4: DSC-4:AC-2

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		
Course Title: SEPARATION METHODS-I **Course Code:** Analytical Chemistry-2 (DSC4:AC-2)	04	02	00	02	Physics, Chemistry and Mathematics	-

Learning Objectives

The Learning Objectives of this course are as follows:

- To acquire basic knowledge of the analytical chemistry of important techniques that will provide the basis for their industrial production methods.
- To provide an adequate mastery of analytical methods used for the determination of commercial/domestic raw materials and finished product quality.

Learning outcomes

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

- Become familiar with fundamental concepts of partition coefficients and their role in achieving separations across different types of chromatography.
- Develop the core skills to parse existing chromatographic protocols and identify the key factors influencing a chromatography experiment.
- Understand the underlying assumptions of the most common chromatographic separation techniques and approaches to method validation.
- Understand the concept of solubility and their application in separation using distribution law.

SYLLABUS OF Analytical Chemistry-2 (DSC-4: AC-2)

Theory Component

UNIT – I: Chromatography (4 Weeks)

Classification of chromatographic methods: Principles of differential migration, description of chromatographic process, distribution coefficients, modes of chromatography. the chromatography (elution time and volume) capacity factor, column efficiency and resolution, sample preparation.

UNIT – II: Techniques of paper chromatography (3 Weeks)

Experimental modifications, various modes of developments, nature of paper, detections of spots, retardation factors, factors that affect reproducibility of R_f values (due to paper, solvent system, sample, development procedures), selection of solvent, quantitative analysis, applications.

UNIT – III: Thin Layer Chromatography (3 Weeks)

Stationary phase, adsorbents, liquid phase support, plate preparation, mobile phase, sample application, development, saturation of chamber, detection of spot, R_f values (effect of adsorbent, solvent, solute, development process), quantitative analysis, applications.

UNIT – IV: Solvent Extraction (2 Weeks)

Distribution law, determination of distribution ratio, batch extraction, continuous extraction, discontinuous extraction, counter-current extraction.

UNIT –V: Dialysis and membrane filtration (3 Weeks)

General laboratory methods, filters-nitrocellulose, fiberglass and polycarbonates.

Practical component

(Credits: 02; Laboratory Periods: 60; 15 Classes of 4 hours each)

1. Separation and identification of amino acids present in the given mixture by **radial** and **ascending** paper Chromatography (*Perform both*).
2. Separation of ortho-nitrophenol & para-nitrophenol and *o*- and *p*-amino phenol by thin layer chromatography (TLC) and calculation of their R_f values.
3. Separation of constituents of leaf pigments by thin layer chromatography and paper chromatography (*radial & ascending both*).
4. Separation of a mixture of compounds by solvent extraction.
5. Separation of a mixture of naphthalene, benzoic acid and 2-naphthol.
6. Separation of a mixture of 1,4-dimethoxybenzene, 2-chloro benzoic acid and *p*-cresol.
7. Analysis of soil samples (*at least three soil samples to be collected for analysis*) collected from college nursery, sports ground Delhi villages/ Yamuna River bank.

   (**a**) Determination of pH of soil samples.
   (**b**) Determination of total soluble salts.
   (**c**) Determination of carbonate and bicarbonate.
   (**d**) Determination of calcium, magnesium and iron.
   (**e**) Determination of conductance of the soil samples.
8. Industrial visit to STP plant.

Essential/recommended readings

- Fifield,F.W.; Kealey, D. (2000), Principles and Practice of Analytical Chemistry, Wiley.
- Harris, D. C. (2007), Exploring Chemical Analysis, W.H. Freeman and Co.
- Harris, D. C. (2007), Quantitative Chemical Analysis, 6th Edition, Freeman
- Mikes, O. (2000), Laboratory Handbook of Chromatographic methods, D.Van Nostrand Company Inc.

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

DISCIPLINE SPECIFIC CORE COURSE – 5: DSC5:C2

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		
Course Title: PERIODIC PROPERTIES AND CHEMICAL BONDING **Course Code:** CHEMISTRY-2 (DSC5-C2)	04	02	00	02	Physics, Chemistry and Mathematics	-

Learning Objectives

The Learning Objectives of this course are as follows:

- The course discusses the periodicity in properties with reference to the s, p and d block, which is necessary in understanding their group chemistry.
- It provides basic knowledge about ionic, covalent and metallic bonding underlining the fact that chemical bonding is best regarded as a continuum between the three cases.
- It provides an overview of hydrogen bonding and van der Waal forces which influence the melting points, boiling points, solubility and energetics of dissolution of compounds.

Learning outcomes

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

- Understand periodicity in ionization enthalpy, electron gain enthalpy, electronegativity and enthalpy of atomization.

- Understand variability in oxidation state, colour, metallic character, magnetic and catalytic properties and ability to form complexes
- Understand the concept of lattice energy using Born-Landé expression.
- Draw Born Haber Cycle and analyse reaction energies.
- Draw the plausible structures and geometries of molecules using VSEPR theory.
- Understand and draw MO diagrams (homo- & hetero-nuclear diatomic molecules).
- Understand the importance and applications of hydrogen and van der Wall bonding.

SYLLABUS OF Chemistry-2 (DSC-5:C2)

Theory Component

UNIT – I: Periodic Properties (6 Weeks)

Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy, inert pair effect.

General group trends of s, p and d block elements with special reference to Ionization Enthalpy, Electron Gain Enthalpy, Electronegativity, Enthalpy of Atomization, oxidation state, colour, metallic character, magnetic and catalytic properties, ability to form complexes.

UNIT – II: Bonding in Coordination Compounds (9 Weeks)

Ionic Bonding: General characteristics of ionic bonding, Lattice Enthalpy and Solvation Enthalpy and their relation to stability and solubility of ionic compounds, Born-Lande equation for calculation of Lattice Enthalpy (no derivation), Born-Haber cycle and its applications, polarizing power and polarizability, Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Covalent Bonding: Valence Bond Approach, Hybridization and VSEPR Theory with suitable examples, Concept of resonance and resonating structures in various inorganic and organic compounds, Molecular Orbital Approach: Rules for the LCAO method, bonding, nonbonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO, NO and NO^+.

Metallic Bonding, Hydrogen Bonding, van der Waals Forces.

Practical component

(Credits: 02; Laboratory Periods: 60; 15 Classes of 4 hours each)

1. Preparation of standard solutions of different normality and molarity of Mohr’s salt and oxalic acid.
2. Estimation of free alkali present in different soaps and detergents (*At least two samples to be taken*).
3. Estimation of oxalic acid by titrating it with $KMnO_4$ (*Provide at least two unknown solutions*).
4. Estimation of Mohr’s salt by titrating it with $KMnO_4$ (*Provide a tleast two unknown solutions*).
5. Estimation of water of crystallization in Mohr’s salt by titrating with $KMnO_4$.
6. Estimation of Fe (II) ions by titrating it with $K_2Cr_2O_7$ using internal and external indicators.
7. Estimation of Cu (II) ions iodometrically using $Na_2S_2O_3$.
8. Chromatographic separation of mixture of metal ions Cu^{2+}, Cd^{2+} and Ni^{2+}, Co^{2+}.

Essential/recommended readings

- Huheey, J.E.; Keiter, E.A., Keiter; R. L.; Medhi, O.K. (2009), Inorganic Chemistry-Principles of Structure and Reactivity, Pearson Education
- Shriver, D.D.; Atkins, P.; Langford, C.H. (1994), Inorganic Chemistry 2nd Ed., Oxford University Press.
- Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), Inorganic Chemistry, 5th Edition, W. H. Freeman and Company.
- Lee, J.D.; (2010), Concise Inorganic Chemistry, Wiley India
- Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994), Concepts and Models of Inorganic Chemistry, John Wiley & Sons.
- Wulfsberg, G (2002), Inorganic Chemistry, Viva Books Private Limited.
- Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), Inorganic Chemistry, 5th Edition, Pearson.
- 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 CORE COURSE – 6: Mathematics-1:DSC6

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		
Course Title: Topics in Calculus **Course Code:** Mathematics-1 (DSC6)	04	**03**	**01**	**00**	**Physics, Chemistry and Mathematics**	**-**

Course Objectives

The Learning Objectives of this course are as follows:

- The primary objective of this course is to introduce the basic tools of calculus which are helpful in understanding their applications in many real-world problems.
- Students will be able to understand/create various mathematical models in everyday life.

Course Learning Outcomes: This course will enable the students to:

- Understandcontinuityanddifferentiabilityintermsoflimitsandgraphsofcertainfunctions.
- Describe asymptotic behaviour in terms of limits involving infinity.
- Use of derivatives to explore the behaviour of a given function locating and classify its extrema and graphing the function.
- Apply the concepts of asymptotes, and inflexion points in tracing of Cartesian curves.
- Compute the reduction formulae of standard transcendental functions with applications.

Theory Component

Unit 1: Limits, Continuity and Differentiability
Limit of a function, $\varepsilon-\delta$ definition of a limit, Infinite limits, Continuity and types of discontinuities; Differentiability of a function, Successive differentiation: Calculation of the *n*th derivatives, Leibnitz theorem; Partial differentiation, Euler's theorem on homogeneous functions.

Unit 2: Mean Value Theorems and its Applications
Rolle's theorem, Mean value theorems and applications to monotonic functions and inequalities; Taylor's theorem, Taylor's series, Maclaurin's series expansions of e^x, $\sin x$, $\cos x$, $\log(1+x)$ and $(1+x)^m$; Indeterminate forms.

Unit 3: Tracing of Curves and Reduction Formulae
Asymptotes (parallel to axes and oblique), Concavity and inflexion points, Singular points, Tangents at the origin and nature of singular points, Curve tracing(cartesian and polar equations). Reduction formulae for $\int \sin^n x\,dx$, $\int \cos^n x\,dx$, and $\int \sin^m x \cos^n x\,dx$ and their applications.

Practical Component (if any): NIL

Essential/recommended readings

- Prasad, Gorakh (2016). *Differential Calculus* (19th ed.). Pothishala Pvt. Ltd. Allahabad.
- Prasad, Gorakh (2015). *Integral Calculus*. Pothishala Pvt. Ltd. Allahabad.

Additional Readings:

- Apostol, T. M. (2007). *Calculus*: *One-Variable Calculus with An Introduction to Linear Algebra* (2nd ed.). Vol. 1. Wiley India Pvt. Ltd.
- Ross, Kenneth. A. (2013).*Elementary Analysis*: *The Theory of Calculus* (2nd ed.).Undergraduate Texts in Mathematics, Springer. Indian reprint.

GE Pool B: Semester II, IV, VI (EVEN SEMESTERS)

1. GE-2: Coordination and Organometallic Compounds
2. GE-5: Chemistry of Oxygen containing Functional Groups and their Application to Biology
3. GE-8: Chemical Kinetics and Photochemistry
4. GE-10: Basics of Polymer Chemistry
5. GE-14: Chemistry: Molecular Modelling, Artificial Intelligence and Machine Learning
6. GE-6: Molecules of Life
7. GE-16: Role of Metals in Medicines
8. GE-17: Energy and the Environment
9. GE-18: Fragrances and Flavours: An Industry’s Perspective
10. GE-20: Green Chemistry

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		
Coordination and Organometallic Compounds (GE-2)	4	2		2		

Learning Objectives

The Learning Objectives of this course are as follows:

- **To introduce students to some important d-block metals and their compounds which they are likely to come across.**
- **To make students learn about organometallic compounds, a frontier area of chemistry providing an interface between organic and inorganic chemistry.**
- To familiarize students with coordination compounds which find manifold applications in diverse fields.

Learning outcomes

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

- Familiarize with different types of organometallic compounds, their structures and bonding involved.
- Understand the nature of Zeise's salt and compare its synergic effect with that of carbonyls.
- Identify important structural features of tetrameric methyl lithium and understand the concept of multicenter bonding in these compounds
- Apply 18-electron rule to rationalize the stability of metal carbonyls and related species
- Use IR data to explain the extent of back bonding in carbonyl complexes
- Understand the terms, ligand, denticity of ligands, chelate, coordination number and use standard rules to name coordination compounds
- Use Valence Bond Theory to predict the structure and magnetic behaviour of metal complexes and understand the terms inner and outer orbital complexes
- Understand the properties of coordination compounds and VBT and CFT for bonding in coordination compounds
- Explain the meaning of the terms Δ_o, Δt, pairing energy, CFSE, high spin and low spin and how
- CFSE affects thermodynamic properties like lattice enthalpy and hydration enthalpy

Theory:

Unit 1: Coordination Chemistry **Lectures: 4**

Brief discussion with examples of types of ligands, denticity and concept of chelate. IUPAC system of nomenclature of coordination compounds (mononuclear and binuclear) involving simple monodentate and bidentate ligands.

Unit 2:Bonding in coordination compounds **Lectures: 14**

Valence Bond Theory (VBT): Salient features of theory, concept of inner and outer orbital complexes of Cr, Fe, Co and Ni. Drawbacks of VBT.

Crystal Field Theory: Splitting of d orbitals in octahedral symmetry. Crystal field effects for weak and strong fields. Crystal field stabilization energy (CFSE), concept of pairing energy. Factors affecting the magnitude of Δ_o.

Spectrochemical series. Splitting of d orbitals in tetrahedral symmetry. Comparison of CFSE for octahedral and tetrahedral fields, tetragonal distortion of octahedral geometry. Jahn-Teller distortion, square planar coordination.

Unit 3: Organometallic Compounds **Lectures: 12**

Definition and classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structure and bonding of methyl lithium and Zeise's salt. Structure and physical properties of ferrocene. 18-electron rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals. π-acceptor behaviour of carbon monoxide (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

Practicals: **Credits: 02**
(Laboratory periods: 60)

1. Gravimetry

Discuss basic principles of gravimetry (precipitation, co- precipitation and post precipitation, digestion, washing etc)

(i) Estimation of Ni(II) using dimethylglyoxime (DMG).

(ii) Estimation of copper as CuSCN.

(iii) Estimation of Al(III) by precipitating with oxine and weighing as Al(oxine)3 (aluminium oxinate).

2. Inorganic Preparations

(i) Schiff's base involving ethylenediamine and salicylaldehyde (or any other amine and aldehyde/ketone) and to check its purity using TLC.
(ii) Nickel/ Copper complex of the above prepared Schiff's base and its characterisation using UV/Vis spectrophotometer. The IR spectra also to be interpreted
(iii) tetraamminecopper (II) sulphate
(iv) potassium trioxalatoferrate (III) trihydrate.

(v) tetraamminecarbonatocobalt(III) nitrate

References:

Theory:

1. 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.
2. Miessler, G. L.; Fischer P.J.; Tarr, D.A. (2014), **Inorganic Chemistry**, Pearson.
3. Huheey, J.E.; Keiter, E.A., Keiter; R.L., Medhi, O.K. (2009), **Inorganic Chemistry-Principles of Structure and Reactivity**, Pearson Education.
4. Pfennig, B. W. (2015), **Principles of Inorganic Chemistry.** John Wiley & Sons.
5. Cotton, F.A.; Wilkinson, G. (1999), **Advanced Inorganic Chemistry** Wiley-VCH.

Practicals:

1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989), **Vogel's Textbook of Quantitative Chemical Analysis**, John Wiley and Sons.
2. Schiff Base Complex of Cu (II) with Antibacterial and Electrochemical Study, Arjun C. Bhowmick, Majharul I. Moim, Miththira Balasingam **, American Journal of Chemistry** 2020, 10(2): 33-37, DOI: 10.5923/j.chemistry.20201002.03

Teaching Learning Process:

- Conventional chalk and board teaching,
- Class interactions and discussions
- Power point presentation on important topics.

Assessment Methods:

- Presentations by Individual Student/ Group of Students
- Class Tests at Periodic Intervals.
- Written assignment(s)
- End semester University Theory and Practical Examination

Keywords: Organometallic compounds, metal carbonyls, synergistic effect, Coordination compounds, VBT, Crystal field theory, Splitting of d levels, Dq

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		
Chemistry of Oxygen containing Functional Groups and their	4	2		2		

Applications to Biology **(GE-5)**						

Learning Objectives

The Learning Objectives of this course are as follows:

- To teach the fundamental chemistry of oxygen containing functional groups.
- To establish these concepts typical reactions of alcohols, phenols, aldehydes, ketones, carboxylic acids and their derivatives.
- To make students understand the relevance of oxygen containing functional groups to biology and the importance of these compounds in real world.

Learning outcomes

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

- Understand and explain the differential behavior of organic compounds based on reaction chemistry.
- Formulate the mechanism of organic reactions by recalling and correlating the fundamental properties of the reactants involved.
- Understand the applications of functional group chemistry to biology.

Theory:

Unit 1: Alcohols (upto 5 Carbon) Lectures: 5

Structure and classification of alcohols as 1°, 2° & 3°, Reactions: Acidic character of alcohols and reaction with sodium, with HX (Lucas Test), esterification, oxidation (with PCC, alkaline $KMnO_4$, acidic $K_2Cr_2O_7$ and conc. HNO_3), Oppeneauer Oxidation, Biological oxidation Reactions

Unit 2: Phenols Lectures: 4

Acidity of phenols and factors affecting their acidity, Reactions: Electrophilic substitution reactions, *viz.* nitration, halogenation, sulphonation, Reimer-Tiemann reaction, Gattermann–Koch reaction, Houben-Hoesch condensation; Reaction due to OH group: Schotten-Baumann reaction

Unit 3: Aldehydes and Ketones (Aliphatic and Aromatic) Lectures: 12

Reactions: Nucleophilic addition, nucleophilic addition-elimination reaction including reaction with HCN, ROH, $NaHSO_3$, NH_2-G derivatives. Iodoform test, Aldol condensation and its biological application, Cannizzaro's reaction, Wittig reaction, Benzoin condensation, Clemmensen reduction, Wolff Kishner reduction, Meerwein-Pondorff Verley reduction, enzyme-catalyzed additions to α,β-unsaturated carbonyl compounds.

Unit 4: Carboxylic acids and their derivatives (Aliphatic and Aromatic) Lectures: 9

Reactions: Hell-Volhard Zelinsky reaction, acidity of carboxylic acids, effect of substitution on acid strength, Claisen condensation and its biological applications, decarboxylation in biological systems, relative reactivities of acid derivatives towards nucleophiles, activation of carboxylate ions for nucleophilic acyl substitution reactions in biological systems, Reformatsky reaction, Perkin condensation.

Practicals: Credits: 02
(Laboratory periods: 60)

Preparations: (Mechanism of various reactions involved to be discussed) (Recrystallization, determination of melting point and calculation of quantitative yields to be done in all cases)

1. Oxime of aldehydes and ketones

2. 2,4-Dinitrophenylhydrazone of aldehydes and ketones

3. Aldol condensation using green method.

4. Benzoin condensation using Thiamine Hydrochloride as a catalyst.

5. Alkaline hydrolysis of amide/ester.

6. Benzoylation of one of the following amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) or one of the following phenols (*β*-naphthol, resorcinol, p-cresol) by Schotten-Baumann reaction.

7. Identification of functional group for monofunctional organic compounds (Alcohols, phenols, aldehydes, ketones, carboxylic acids).

References:
Theory:

1. Sykes, P. (2005), **A Guide Book to Mechanism in Organic Chemistry**, Orient Longman.
2. Eliel, E. L. (2000), **Stereochemistry of Carbon Compounds**, Tata McGraw Hill.
3. Morrison, R. N.; Boyd, R. N., Bhattacharjee, S.K. (2010), **Organic Chemistry**, 7th Edition, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Mehta B.; Mehta M. (2015), **Organic Chemistry**, PHI Learning Private Limited Bahl,
5. Bahl, A., Bahl, B. S. (2012), **Advanced Organic Chemistry**, S. Chand.
6. Bruice, Paula Y. (2020), **Organic Chemistry**, 8th Edition, Pearson.

Practicals:

1. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. (2012), **Vogel's Textbook of Practical Organic Chemistry**, Pearson.
2. Mann, F.G.; Saunders, B.C. (2009), **Practical Organic Chemistry**, Pearson Education.

Teaching Learning Process:

- Lectures in class rooms

- Power point presentations/videos
- Hands-on learning using 3-D models

Assessment Methods:

- Presentation/assignment by students
- Class Test at Periodic Intervals
- Written Assignment
- Continuous evaluation in practicals
- End Semester University Theory and Practical Exams

Keywords: Alcohols, Lucas Test, Phenol, Aldehydes, Ketones, Nucleophilic addition, nucleophilic addition – elimination, Cannizzaro's reaction, Wittig reaction, Benzoin condensation, Enzyme-catalysed reaction, Carboxylic acid, Claisen condensation

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		
Molecules of Life (GE-6)	4	2		2		

Learning Objectives

The Learning Objectives of this course are as follows:

- To deliver information about the chemistry of carbohydrates, proteins & enzymes and its relevance in the biological system using suitable examples.
- To place key emphasis on understanding the structural principles that govern reactivity/physical /biological properties of biomolecules as opposed to learning structural details.

Learning outcomes

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

- Learn and demonstrate how the structure of biomolecules determines their chemical properties, reactivity and biological uses.
- Gain an insight into the mechanism of enzyme action and inhibition.
- Understand the basic principles of drug-receptor interaction and SAR.

Theory:

Unit 1: Carbohydrates **Lectures: 12**

Classification of carbohydrates, reducing and non-reducing sugars, biological functions, general properties and reactions of glucose and fructose, their open chain structure, epimers, mutarotation and anomers, reactions of monosaccharides, determination of configuration of glucose (Fischer proof), cyclic structure of glucose. Haworth projections. Cyclic structure of fructose. Linkage between monosaccharides: structure of disaccharides (sucrose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

Unit 2: Amino Acids, Peptides and Proteins Lectures: 10

Classification of amino acids and biological uses of amino Acids, peptides and proteins. Zwitterion structure, isoelectric point and correlation to acidity and basicity of amino acids. Determination of primary structure of peptides, determination of N-terminal amino acid (by Edman method) and C– terminal amino acid (with carboxypeptidase enzyme). Synthesis of simple peptides (up to dipeptides) by N-protection (t-butyloxycarbonyl) & C-activating groups (only DCC) and Merrifield solid phase synthesis, Overview of primary, secondary, tertiary and quaternary structure of proteins, denaturation of proteins.

Unit 3: Enzymes and correlation with drug action Lectures: 8

Classification of enzymes and their uses (mention Ribozymes). Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (Competitive and non-competitive inhibition including allosteric inhibition). Drug action-receptor theory. Structure – activity relationships of drug molecules, binding role of –OH group, -NH_2 group, double bond and aromatic ring.

Practicals: Credits: 02

(Laboratory periods: 60)

1. Estimation of glucose by Fehling's solution.
2. Determination of total sugar content by ferricyanide method (volumetric/colorimetric method).
3. Study of the titration curve of glycine.
4. Estimation of proteins by Lowry's method.
5. Study of the action of salivary amylase on starch under optimum conditions.
6. Qualitative tests for amino acids, proteins and carbohydrates.
7. Separation and identification of mixture of sugars by paper chromatography.

References:

Theory:

1. Finar, I. L. **Organic Chemistry** (Volume 1 & 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Morrison, R. N.; Boyd, R. N., Bhattacharjee, S.K. (2010), **Organic Chemistry**, 7th Edition, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Berg, J. M.; Tymoczko, J. L.; Stryer, L. (2019), **Biochemistry**, 9th Ed., W. H. Freeman Co Ltd.

Practicals:

1. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. (2012), **Vogel's Textbook of Practical Organic Chemistry**, Pearson.
2. **Manual of Biochemistry Workshop**, 2012, Department of Chemistry, University of Delhi.

Teaching Learning Process:

- Chalk and black board method. Along with pedagogy of flipped classroom
- Certain topics like mechanism of enzyme action and enzyme inhibition can be taught through audio-visual aids.
- Students should be encouraged to participate actively in the classroom through regular presentations on curriculum-based topics, peer assessment, designing games based on specific topics etc.
- As the best way to learn something is to do it yourself, practicals are planned in such a way so as to reinforce the topics covered in theory.

Assessment Methods:

- Graded assignments
- Class tests and Quizzes
- Class seminars by students on course topics with a view to strengthening the content through width and depth
- Continuous evaluation for the practicals
- End semester university theory and practical examination.

Keywords: Carbohydrates, point, Amino acids, Enzymes, SAR, Drug Receptor Theory

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		
Chemical Kinetics and Photochemistry (GE-8)	4	2		2		

Learning Objectives

The Learning Objectives of this course are as follows:

- To make students learn about the fundamentals of chemical kinetics, rates of chemical reactions, complex reactions, theories of reaction rate and the laws of photochemistry aimed at understanding electronic transitions upon irradiation of electromagnetic radiation in UV-Vis region.

Learning outcomes

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

- Understand the concept of rate of a reaction, order and molecularity of a reaction, various factors affecting the rate and theories of reaction rates.
- Students will be able to apply the learnt concepts in studying the reaction kinetics of various reactions.
- Understand the basic concepts of photochemistry, photochemical and photosensitized reactions and their role in biochemical systems.

Theory:

Unit 1: Chemical Kinetics — Lectures: 20

The concept of reaction rates, effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction, derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants), half–life of a reaction, general methods for determination of order of a reaction. kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms). Concept of activation energy and its calculation from Arrhenius equation. Theories of reaction rates: Collision theory and activated complex theory of bi-molecular reactions. Comparison of the two theories (qualitative treatment only)

Unit 2: Photochemistry — Lectures: 10

Characteristics of electromagnetic radiation, Jablonski Diagram. Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitized reactions, quenching. Role of photochemical reactions in biochemical processes.

Practicals: — Credits: 02

(Laboratory periods: 60)

Chemical Kinetics

Study the kinetics of the following reactions by integrated rate method:

a) Acid hydrolysis of methyl acetate with hydrochloric acid.

b) Compare the strength of HCl and H2SO4 by studying the kinetics of hydrolysis methyl acetate.

c) Initial rate method: Iodide-persulphate reaction

d) Integrated rate method: Saponification of ethyl acetate.

e) Study the reactiob kinetics of Iodination of acetone.

References:

Theory:

1. Castellan, G.W. (2004), **Physical Chemistry**, Narosa.

2. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 5, 6th Edition, McGraw Hill Education.

3. Kapoor, K.L. (2013), **A Textbook of Physical Chemistry**, Vol 6, 3rd Edition, McGraw Hill Education.

Practicals:
1. Khosla, B.D.; Garg, V.C.;Gulati, A.(2015), **Senior Practical Physical Chemistry**, R. Chand & Co.

Teaching Learning Process:

- Teaching Learning Process for the course is visualized as largely student-focused
- Transaction through an intelligent mix of conventional and modern methods
- Engaging students in cooperative learning.
- Learning through quiz design.
- Problem solving to enhance comprehension.

Assessment Methods: Assessment will be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

Keywords: Rate Law, Rate constant. Arrhenius Equation, Lambert-Beer's law, Jablonski Diagram

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		
Basics of Polymer Chemistry **(GE-10)**	4	2		2		

Learning Objectives

The Learning Objectives of this course are as follows:
- To help the student to know about the synthesis, properties and applications of polymers.

Learning outcomes

By the end of the course, the students will be able to:
- Know about classification of polymeric material.
- Learn about different mechanisms of polymerization and polymerization techniques
- Evaluate kinetic chain length of polymers based on their mechanism
- Differentiate between polymers and copolymers
- Learn about different methods of finding out average molecular weight of polymer.
- Differentiate between glass transition temperature (Tg) and crystalline melting point (Tm)
- Learn properties and applications of various useful polymers in our daily life

Theory:

Unit 1: Introduction to polymers
Lectures:10

Different schemes of classification of polymers, Polymer nomenclature, configuration and conformation of polymers, Molecular forces and chemical bonding in polymers, Texture of Polymers

Functionality and its importance:

Criteria for synthetic polymer formation, basic methods of polymerization processes and their mechanism: addition, condensation, Relationships between functionality, extent of reaction and degree of polymerization.

Unit 2: Properties of Polymers **Lectures: 10**

Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg).

Crystallization and crystallinity: Determination of crystalline melting point and degree of crystallinity,

Morphology of crystalline polymers, Factors affecting crystalline melting point.

Molecular weight distribution and determination of molecular weight of polymers (Mn, Mw, etc.) by end group analysis, viscometry and osmotic pressure methods. Molecular weight distribution and its significance.

Unit 3: Preparation, properties and applications **Lectures: 10**

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride), poly(vinyl acetate), acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novolac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers: polyacetylene, polyaniline, poly(p-phenylene sulphide, polypyrrole, polythiophene

Practicals: **Credits: 02**

(Laboratory periods: 60)

Polymer Synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA)/MethylAcrylate (MA).
2. Preparation of nylon 6,6
3. Redox polymerization of acrylamide
4. Precipitation polymerization of acrylonitrile
5. Preparation of urea-formaldehyde resin
6. Preparations of novalac resin/resole resin.
7. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

1. Determination of molecular weight of polyvinyl propylidene in water by viscometry.
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of head-to-head monomer linkages in the polymer.

3. Determination of molecular weight by end group analysis of polymethacrylic acid.

Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method.
2. Determine the melting point of crystalline polymer.
3. Measurement of glass transition temperature, T_g.s

References:

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. Ghosh, P. (2001), **Polymer Science & Technology**, Tata Mcgraw-Hill.
5. Lenz, R.W. (1967), **Organic Chemistry of Synthetic High Polymers**, Intersecience (Wiley).

Practical:

1. Allcock, H.R.; Lampe, F. W.; Mark, J. E. (2003), **Contemporary Polymer Chemistry**, Prentice-Hall.
2. Fried, J.R. (2003), **Polymer Science and Technology**, Prentice-Hall.
3. Munk, P.; Aminabhavi, T. M. (2002), **Introduction to Macromolecular Science,** John Wiley & Sons.
4. Sperling, L.H. (2005), **Introduction to Physical Polymer Science**, John Wiley & Sons.

Teaching Learning Process:

- Student centred teaching Learning process.
- Blend of conventional blackboard teaching and modern teaching learning tools
- Focus on real life applications of concepts
- Problem solving and quizzes for enhanced understanding of the concepts
- Engaging students in collaborative learning.
- Pre-lab learning of theoretical concept of the experiment.
- Performing the experiment, recording the data, calculating the result.
- Interpreting the result.
- Comparing the results of the class.
- Discussing the sources of error.

Assessment Methods:

- Class Tests at Periodic Intervals.
- Written assignment(s)
- Continuous evaluation of laboratory work and record file.
- Oral assessment, quizzes.
- Mock practical examination.
- Semester end University examination.

Keywords: Bonding, Texture, Polymerization, Crystallization, Properties, Applications.

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		
Molecular Modelling, Artificial Intelligence and Machine Learning in Chemistry **(GE-14)**	**4**	**2**		**2**		

Learning Objectives

The Learning Objectives of this course are as follows:

- To make students familiarize with modern scientific machine (programming) language i.e., Python, artificial intelligence (AI) & machine learning (ML) and their potential applications in chemistry.
- To provide elementary ideas of the techniques prevailing in the field of artificial intelligence (AI) and machine learning (ML) and their applications to research problems especially related to research and development of new materials and pharmaceutical compounds with desired properties.

Learning outcomes

By the end of the course, the students will be:

- Conversant with the Python Programming Language.
- Familiar with Elementary techniques of Artificial intelligence (AI) & Machine learning (ML)
- Able to apply techniques of AI & ML in basic problems of research in some important areas of research in Chemistry.

Theory:

Part A: Molecular Modelling

Introduction to computational chemistry: **Lectures: 7**

Overview of Computational Methods in Chemistry (Ab initio, DFT, Semi- empirical, Molecular Mechanics

Potential Energy Surfaces **Lectures: 4**

The concept of Potential energy surface, Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global minima, Geometry optimization and energy minimization.

Molecular Mechanics **Lectures: 4**

Force Fields (A brief idea of a basic force field), Elementary idea of MM1, MM2, MM3, MM4, MM+, AMBER etc. A brief Idea of Molecular Docking

Part B: Artificial Intelligence & Machine learning in Chemistry **Lectures: 15**

An overview of computationally readable and processible representation of molecules, e.g., SMILES, mol files. Chemical space and access to chemical databases. Statistical treatment of data: regression analysis and types of regression. Elementary Idea of Quantitative structure-activity relationship (QSAR).

An insight into Artificial Intelligence & Machine learning and potential areas of applications in chemistry. Dimensional reduction; Principal Component Analysis (PCA) and the importance and necessity of nonlinearity in Artificial Intelligence.

Genetic algorithm, basics of random mutation hill climbing (RMHC) and simulated annealing.

Practicals/Hands-on Training: **Credits: 02**

(Laboratory periods: 60)

Molecular Modeling based Exercise

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

2) Carry out geometry optimisation on H_2O, H_2S, H_2Se molecules and 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 mechanicalmethods.

3) Calculate the energy of the following chemical species andarrange 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 the geometry optimisation on the following chemical species and compare the shapes and dipole moments of the molecules.

1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2- propanol.

Correlate the computationally obtained values of the dipole moments with the experimental values of the boiling points: (118ºC, 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 Ethene.

6) Based on the calculations of enthalpies 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)

$$N_2 + 3\,H_2 \rightarrow 2NH_3$$ (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 optimization & 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:

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

11) QSAR based exercise on problems of interest to chemist.

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

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

14) 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.

15) 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.

16) Perform molecular docking of Sulfonamide-type D-Glu inhibitor into MurD active site using Argus lab.

Artificial Intelligence (AI) and Machine Learning (ML) based exercise on problems of interest to chemist

17. Travelling salesman problem and electrical circuit design (minimization of path-length).
18. Genetic algorithm, in solving matrix form of linear equations
19. Non-linear least-square fitting problem.
20. Particle Swarm Optimization on the sphere function.

Important Instruction Note on working approach:

- A student is required to perform/investigate a minimum of 10 exercises in total.
- The exercises mentioned above will be performed by the student strictly in accordance with the instructions received and only under the supervision of the teacher concerned.
- Any other exercise may be carried out with prior permission, input, discussion and instructions received from the teacher concerned.

References:

1. Lewars, E. (2003), **Computational Chemistry**, Kluwer academicPublisher.
2. Cramer, C.J. (2004), **Essentials of Computational Chemistry**, John Wiley & Sons.
3. Cartwright C.; Kharma N., (2008), **Using artificial intelligence in chemistry and biology**, First Edition, CRC Press Taylor & Francis Group
4. Hippe; Z., **Artificial Intelligence in Chemistry: Structure Elucidation and Simulation of Organic Reactions**, (1991) Academic Press, Elsevier
5. Soft Computing in Chemical and Physical Sciences A Shift in Computing Paradigm (Kanchan Sarkar, Sankar Prasad Bhattacharyya) (z-lib.org)
6. Understanding Properties of Atoms, Molecules and Materials (PRANAB. SARKAR, Sankar Prasad Bhattacharyya) (z-lib.org)

Web Resources:

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/

Teaching Learning Process: Hands-on laboratory exercises Conventional teaching learning method. Engaging students in collaborative learning

Assessment Methods:

- Continuous evaluation of laboratory work and record file.Oral assessment, quizzes.
- Presentation on lab practices.Semester end examination.

Keywords: Molecular Modeling, Potential Energy Surface (PES), Geometry Optimization, Frequency calculation, Artificial Intelligence, Machine Learning, Nural Networks, Genetic Algorithm.

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		
Role of Metals in Medicines **(GE-16)**	**4**	**2**		**2**		

Learning Objectives

The Learning Objectives of this course is as follows:

- To make the learners familiar about role of metal ions in some commercially available medicines.

Learning outcomes

By the end of this course student will be able to learn:

- Role of metal ions in various biomolecules and their functions.
- Role of metals in commercially available medicines and their functions

Theory:

Unit 1: Bio role of Metals Lectures: 4

Brief introduction of following metals in biological system
Fe, Cu, Zn, Mn, Cr(III), V, Mo, W, Co, Ni, Na, K, Mg and Ca
Chemical structure, Commercial name, Name of the disease it is made for and its brief mechanism of action shall be taught for all the mentioned metals below.

Unit 2: Diagnostic and therapeutic agents Lectures: 8

Diagnostic and therapeutic agents with Pt (Cisplatin) and Ga for cancer, Au (auranofin) for arthritis and V for diabetes.

Unit 3: Metals in drugs Lectures:6

Li_2CO_3 (Camcolit) for manic-depressive illness, $NaHCO_3$ (Alka-seltzer) for heartburn, $Al(OH)_3$ (Gaviscon) for heartburn, As (melarsoprol) for sleeping sickness, Bi subsalicylate (pepto-Bismol) for heartburn and diarrhea, Bi subcitrate (De-nol) peptic ulcer, Zinc oxide with Fe_2O_3 (Calamine lotion) as antimicrobial agent.

Unit 4: Metals in Multivitamins Lectures:6

Cyanocobalamin (Co), Ferrous fumerate (Fe), Magnesium oxide (Mg), Zinc Sulfate (Zn), Manganese sesulphate (Mn), Copper Sulfate (Cu), Sodium selenite (Se) and Chromium trichloride (Cr).

Unit 5: Radiopharmaceuticals and MRI contrast agents Lectures:6

^{99m}Tc for heart, brain and bone imaging, ^{123}I radiopharmaceuticals, $BaSO_4$for X-ray contrast agent, Gd (III) for MRI contrast agents.

Practicals: Credits: 02

(Laboratory periods: 60)

Volumetric titrations:

1. To estimate the acidity of commercially available antacids.

2. To estimate the concentration of Fe in commercially available medicines.
3. To estimate the concentration of Ca in commercially available medicinces.
4. To estimate the strength of carbonate in tablets containing Li_2CO_3
5. To estimate the sodium bicarbonate in synthetic/commercially available drug.
6. To estimate the zinc and iron present in Calamine lotion.
7. To estimate the Mg present in multivitamins.

References:

1. **Metals in Medicine**, John Wiley & Sons Ltd, Nov 2009
2. Chapter-9, **Metals in Medicine**, Stephen J. Lippard
3. Jones, Chris and Thornback, John, **Medicinal applications of coordination chemistry**, Cambridge, UK: Royal Society of Chemistry, 2007

Teaching Learning Process:

- Hands-on laboratory exercises
- Conventional teaching learning method. Engaging students in collaborative learning

Assessment Methods:

- Continuous evaluation of laboratory work and record file. Oral assessment, quizzes.
- Presentation on lab practices.
- Semester end examination.

Key words: Diagnostic, therapeutic agents, multivitamins, radiopharmaceuticals and MRI contrast agents.

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		
Energy and the Environment (GE-17)	4	3		1		

Learning Objectives

The Learning Objectives of this course is as follows:

- To develop basic understanding of energy, issues related to energy, importance of energy in terms of economy, health and the environment.
- To understand different sources of energies, renewable and non-renewable sources of energy. To understand the importance of green fuels.
- To make the students understand the adverse effect of pollution, and possible remediations.

Learning Outcomes

By the end of this course student will be able to learn:

- Describe basic energy concepts
- Account for conventional and renewable energy technologies and their application
- Reflect and evaluate the environmental impact of energy production and the relationship between energy production, consumption and climate change
- Reflect on energy costs, analyse the consequences of today's energy consumption
- Efficient use of energy, water and other resources, Use of renewable energy, such as solar energy
- Pollution and waste reduction measures, and the enabling of re-use and recycling
- Good indoor environmental air quality, Use of materials that are non-toxic, ethical and sustainable
- Consideration of the environment in design, construction and operation

Theory:

Unit 1: **Lectures: 13**

Introduction, chemistry and energy, conversion of chemical energy to electrical energy, Carbon cycle, Greenhouse gases, Global warming and climate change, Carbon footprint, zero-carbon or low-carbon energy. Electrical energy and steam energy, Energy Alternatives, Hidden Costs of Energy.

Unit 2: **Lectures: 10**

Production methods for electric power: Non-Renewable (conventional) sources of energy: Fossil fuels: Coal, petroleum and Natural gas. Energy transformation. Renewable energy sources: solar, hydropower, wind, geothermal, wave, ocean thermal, tidal, ocean currents, nuclear energy, biomass.

Unit 3: **Lectures: 12**

Production methods for electric power: Renewable (green) energy, conversion and storage systems. Nuclear fusion, Hydrogen fuels, photovoltaic solar cells, hydroelectric. Sustainable energy, biomass, Biofuels, production of biofuels, advantages, blending of biofuels with conventional fuels, Carbon Capture and Reuse, Waste to Energy Technologies.

Unit 4: Lectures: 10

Air Pollution, Urban and Indoor Air Pollution, Pollution and waste reduction measures, chemical remediation of air pollution. Effect of pollution on health and economy.

Practicals: **Credits: 01**

(Laboratory periods: 30)

Tutorials

1. Conversion of biomass to biofuels (2-3 different biofuels)

2. Working on solar cell model.
3. Working on wind turbine model.
4. Working on geothermal energy model.
5. Working on hydroelectric plant model.
6. Presentations by students

References:

Theory

1. Rao, C S., **Environment pollution control Engineering**, New Age International reprint 2015, 2nd edition
2. Bharucha, E., **Textbook of Environmental Studies**, Universities Press (2005)
3. Wright, R.T., **Environmental Science-Towards a sustainable Future**, Prentice Hall (2008) 9th edition.
4. Ahluwalia, V. K., **Energy and Environment**, The Energy and Resources Institute (TERI) (2019).

References:

Practicals

- Challapalli Narayan Rao, **Practical approach to implementation of Renewable Energy Systems,** Evincepub Publishing, 2022

Teaching Learning Process: To accomplish a goal, it is very important to learn in a strategic manner. There are different components of learning and the capacity of each learner varies. It is expected to have a student centric teaching. Questions and answers, both should come from students. 'How' to teach and 'What' to teach in the defined curriculum not only depends on the content and the knowledge of the teacher but critically more so on designing, i.e. how to introduce the concept to the students in a very effective way. Different ways of teaching include classical board teaching method, visual conceptual method, application based practical demonstration of the concept etc. are required in this course. In fact, the pedagogy is to make a class interesting and thus learning becomes enjoyable.

Assessment Methods: The effectiveness of learning can be judged by assessing the students. Various types of assessment methods can be followed depending on the branch of student opting the course. Assessment can be in form of Graded assignments, conventional class tests, class seminars and presentations by students on course topics with a view to strengthening the content through width and depth, end semester university examination for theory and practical.

Keywords: Energy, Renewable and non-renewable energy resources, Synthetic fuels, Biofuels, Carbon footprint, air pollution, remediation, pollution related health and economy.

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		
Fragrances and Flavours: An Industry's	**4**	**3**		**1**		

Perspective (GE-18)						

Learning Objectives

The Learning Objectives of this course is as follows:

- To make the students understand the applications of chemistry in the world of flavours and fragrances. The use of fragrance is ubiquitous and is a global human phenomenon. Over the course of time, countless numbers of flavors and fragrances have found their way into everyday life, notably into foods, beverages and confectionery items; into personal care products (soaps, toothpastes, mouthwashes, deodorants, bath lotions and shampoos), perfumes, and other cosmetics as well as pharmaceutical formulations. Indeed, flavors and aromas are added to make such products more attractive or to mask the taste or smell of less pleasant ones.

Learning Outcomes

By the end of this course student will be able to learn:

- Synthesis of various fragrance and flavour ingredients
- Formulation methods, how different factors affects the formulation process in Fragrance and Flavour industry
- Uphold safety regulation and execute quality processes
- Quality control in manufacturing process, legal aspects, classification of odour and odorants.

Different methods used for separation, purification and isolation of perfumes and flavours like distillation, extraction, crystallization, etc.

Theory:

Unit 1: Fragrances **Lectures: 18**

- Introduction to fragrances, types of fragrances (Fragrance families and classification)
- History of perfumes, Perfumery raw materials, classification of odour, odour type and odorants
- India in the context of Fragrance Industry
- ABCs of perfumery, odour aspects of perfumes, fragrance pyramid, fragrance families
- Some basic chemical knowledge to provide a better understanding of the structure of molecules possessing a sensory power, The volatility and solubility of sensory molecules
- Chemistry of aromatic compounds in perfume making, Composition of fragrances
- Current trends in fragrances, sensory analysis of different products
- Study of the raw materials used in perfumery (origin, extraction method, and olfaction)
- Key chemical reactions for conversion of raw materials to fragrances
- Extraction of essential oils used in perfumery
- Difference between alcohol and oil-based perfumes
- Outline of health, safety and sustainability parameters in perfumer

Unit 2: Sustainable Fragrance by Design **Lectures: 4**

- The challenges of sustainability and how it impacts the industry
- Sustainability charter
- Green chemistry principles
- Commitment to Biodiversity

Unit 3: Flavours **Lectures: 18**

- Introduction to flavours, types of flavours, flavour raw materials
- Understanding of terms like, Flavour and Flavouring agents. Attributes of flavour, taste, odour, odour stimulation, basic tastes and the human olfactory system.
- Stability of flavour in food, sensory evaluation of flavours in foods, Various flavour formulation
- Systematic approach to understanding flavour formation during food processing, food matrix, interaction of added flavours
- Flavour enhancers, modifiers, precursors, suppressors, solvents.
- Key chemical reactions for conversion of raw materials to flavours
- Forms of flavour and the manufacturing processes involving all types of flavours. Aroma recovery during processing.
- Biogenesis of flavours in fruits and vegetables, reaction flavours, off flavours.
- Stability of flavor in food, sensory evaluation of flavours in foods
- Selection and application of flavours in foods and beverages
- Legal aspects (natural flavours and natural flavouring substances, nature identical flavouring substances, artificial flavouring substances), and the FSSA act.

Unit 4: Extraction, Isolation and Purification of Perfumes and Flavour Compounds **Lectures: 5**

- Extraction techniques for the separation of volatile oils from natural source- including. Distillation, Evaporation, Crystallization and Adsorption, supercritical fluid extraction methods of isolation of important ingredients

Practicals: **Credits: 01**

(Laboratory periods: 30)

1. Extraction of D-limonene from orange peel using liquid CO_2.
2. Extraction of caffeine from coffee beans using liquid CO_2.
3. Extraction of essential oils from lemon using steam distillation
4. Extraction of essential oils from lemon using liquid CO_2.
5. Extraction of essential oils from fragrant flowers.
6. Determination of esters by Thin Layer Chromatography
7. Memorisation of different raw materials used in perfumery, perfume language, Memorisation of perfumes
8. Testing up of different flavours
9. Analysis of spectra of perfume formulations.

References:

1. Arctander, S. (2008), **Perfume and flavour materials of Natural origin,** Allured Publishing Corporation, USA
2. Arctander, S. (2017), Volume I and II, **Perfume and Flavour Chemicals**, (Aroma Chemicals), Allured Publishing Corporation, USA
3. Curtis,T.; Williams, D. C.(2001) 2nd Edition, **An Introduction to Perfumery**, Micelle Press, USA.
4. Sell,C. (2008), **Understanding Fragrance Chemistry,** Allured Publishing Corporation, USA
5. Calkin,R.R., Jellinek, J.S., **Perfumery: Practice and Principles,** John Wiley & Sons Inc.
6. Gimelli, S.P. (2001), **Aroma Science,** Micelle Press, USA
7. Arctander, S. (2019), **Perfume and Flavour Materials of Natural Origin,** Orchard Innovations
8. https://www.beyondbenign.org/lessons/essential-oil-extraction-using-liquid-co2/

Teaching Learning Process: Blackboard, Power point presentations, Assignments, Field Trips to Flavour and perfumery Industry, Different working models, ICT enabled classes, Interactive sessions, recent literature using internet and research articles.

Assessment Methods: Students' evaluation will be done on the basis of regular class test, presentations and assignments as a part of internal assessment during the course as per the curriculum. End semester university examination will be held for both theory and practical. In practical, assessment will be done based on continuous evaluation, performance in the experiment on the date of examination and viva voce.

Keywords: Fragrances, Flavours, pharmaceutical formulation, distillation, extraction techniques

Course title & Code	**Credits**	**Credit distribution of the course**			**Eligibility criteria**	**Pre-requisite of the course**
		Lecture	**Tutorial**	**Practical/ Practice**		
Green Chemistry **(GE-20)**	**4**	**2**		**2**		

Learning Objectives

The Learning Objectives of this course is as follows:

Huge rise in environmental pollution, depleting resources, climate change, ozone depletion, heaps and heaps of landfills piling up has forced the society to become more and more environmentally conscious. Future chemists and innovators are compelled to work towards sustainable practices. Green chemistry has arisen from these concerns. It is not a new branch of chemistry but helps to improve the creative and innovative thinking in undergraduate students. Green chemistry is a way to boost profits, increase productivity and ensure sustainability with absolute zero waste. Innovations and applications of green chemistry in education have helped companies to gain environmental benefits as well as to achieve economic and societal goals also. Undergraduate students are the ultimate scientific community of tomorrow. Training them to practice chemistry in the safest way possible is key towards safe working conditions in the laboratories as well as the chemical industry and extends to society in a sustainable future for the planet.

Learning Outcomes:

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

- Understand the twelve principles of green chemistry and also 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
- Appreciate the use of catalyst over stoichiometric reagents
- Learn to use green solvents, renewable feedstock and renewable energy sources for carrying out safer chemistry
- Appreciate the use of green chemistry in problem solving skills and critical thinking to innovate and find solutions to environmental problems.
- Learn to design safer processes, chemicals and products through understanding of inherently safer design (ISD)
- Appreciate the success stories and real-world cases as motivation for them to practice green chemistry

Unit 1: Introduction **Lectures:08**

Definition of green chemistry and how it is different from conventional chemistry and environmental chemistry.

• Need of green chemistry

• Importance of green chemistry in- daily life, Industries and solving human health problems (four examples each).

• A brief study of Green Chemistry Challenge Awards (Introduction, award categories and study about five last recent awards).

Unit 2: Twelve Principles of Green Chemistry **Lectures: 12**

The twelve principles of the Green Chemistry with their explanation, Special emphasis on the following:

• Prevention of waste / byproducts, pollution prevention hierarchy.

• Green metrics to assess greenness of a reaction: environmental impact factor, atom economy and calculation of atom economy.

• Green solvents-supercritical fluids, water as a solvent for organic reactions, ionic liquids, solvent less reactions, solvents obtained from renewable sources.

• Catalysis and green chemistry- comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.

• Green energy and sustainability.

• Real-time analysis for pollution prevention.

• Prevention of chemical accidents, designing greener processes, inherent safer design, principle of ISD "What you don't have cannot harm you", greener alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation

Unit 3: **Lectures: 10**

The following Real-world Cases in green chemistry should be discussed: Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments. Designing of environmentally safe marine antifoulant. Rightfit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments. An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn.

Practical: **Credits: 02**

(Laboratory periods: 60)

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 CO_2 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.

References:

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.

Practical:

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**, 4^{th} 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.

Teaching Learning Process:

- *Conventional chalk and board teaching*
- Power point presentations
- Interactive sessions on recent green chemistry presidential awards
- Visit a chemical industry and ask the students to think critically for improving the conditions there.
- Screening of documentaries based on chemical accidents/ and then ask them to think about the solutions

Assessment Methods:

- Presentation/assignment by students
- Class Test at Periodic Intervals
- Written Assignment
- Continuous evaluation in practicals
- End Semester University Theory and Practical Exams

Keywords: Green chemistry, Twelve principles of green chemistry, Atom economy, Waste minimization, green metric, green solvents, Solvent free, Catalyst, Bio-catalyst, Renewable energy sources, Hazardous, Renewable feedstock, Ionic liquids, Supercritical fluids, Inherent safer design, green synthesis, combinatorial, Sustainable development, Presidential green chemistry awards.