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DEPARTMENT OF CHEMISTRY SEMESTER – II

B.SC. (Hons.) Chemistry

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DISCIPLINE SPECIFIC CORE COURSE -4 (DSC-4): CHEMISTRY OF S- AND P-BLOCK ELEMENTS

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		
Chemistry of s- and p-Block Elements (DSC-4: Inorganic Chemistry - II)	04	03	--	01	Class 12 th with Physics, Chemistry, Mathematics	

Learning objectives

The objectives of this course are as follows:

- To develop the general principles of metallurgy and s-, p-block elements.
- To introduce the terms minerals, ores, concentration, benefaction, calcination, roasting, refining, etc. and explain the principles of oxidation and reduction as applied to the extraction procedures.
- To make students ware of different methods of purification of metals, such as electrolytic, oxidative refining, VanArkel-De Boer process and Mond's process are discussed and applications of thermodynamic concepts like that of Gibbs energy and entropy to the extraction of metals.
- To familiarize students with the patterns and trends exhibited by s- and p-block elements and their compounds with emphasis on synthesis, structure, bonding and uses.
- To impart information about the fundamentals of internal and external redox indicators, and iodometric/iodimetric titrations.

Learning outcomes

By studying this course, students will be able to:

- Explain the fundamental principles of metallurgy as well as the importance of recovery of by-products during extraction.
- Apply thermodynamic concepts like that of Gibbs energy and entropy to the principles of extraction of metals.
- Describe the characteristics of s- and p- block elements and apply them for synthesis.
- Apply the concept and use of internal and external redox indicators
- Explain the theory and application of iodometric and iodimetric titrimetric analysis.

SYLLABUS OF DSC-4

UNIT – 1: General Principles of Metallurgy (2 Weeks)

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy with reference to cyanide process for silver and gold. Methods of purification of metals: Electrolytic process, Van Arkel-De Boer process, Zone refining. Brief discussion of metals and alloys used in ancient and medieval India.

UNIT – 2: Chemistry of s-Block Elements (5 Weeks)

General characteristics: melting point, flame colouration, reducing nature, diagonal relationships and anomalous behavior of first member of each group. Reactions of alkali and alkaline earth metals with oxygen, hydrogen, nitrogen and water.

Common features such as ease of formation, thermal stability, energetics of dissolution, and solubility of the following alkali and alkaline earth metal compounds: hydrides, oxides, peroxides, superoxides, carbonates, nitrates, sulphates.

Complex formation tendency of s-block elements; structure of the following complexes: crown ethers and cryptates of Group I; basic beryllium acetate, beryllium nitrate, EDTA complexes of calcium and magnesium.

Solutions of alkali metals in liquid ammonia and their properties

UNIT – 3: Chemistry of p-Block Elements (3 Weeks)

Electronic configuration, atomic and ionic size, metallic/non-metallic character, melting point, ionization enthalpy, electron gain enthalpy, electronegativity, Catenation, Allotropy of C, P, S; inert pair effect, diagonal relationship between B and Si and anomalous behaviour of first member of each group.

UNIT – 4: Compounds of p-Block Elements (5 Weeks)

Acidic/basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, action of heat on the following:

- Hydrides of Group 13 (only diborane), Group 14, Group 15 (EH_3 where E = N, P, As, Sb, Bi), Group 16 and Group 17.
- Oxoacids of phosphorus, sulphur and chlorine
- Interhalogen and pseudohalogen compound
- Clathrate compounds of noble gases, xenon fluorides (MO treatment of XeF_2).

Practical component

1. Redox Titrations

- (i) Estimation of Fe(II) with $\text{K}_2\text{Cr}_2\text{O}_7$ using diphenylamine as internal indicator.
- (ii) Estimation of Fe(II) with $\text{K}_2\text{Cr}_2\text{O}_7$ using N-phenyl anthranilic acid as internal indicator.
- (iii) Estimation of Fe(II) with $\text{K}_2\text{Cr}_2\text{O}_7$ using external indicator.

2. Iodo/Iodimetric Titrations

- (i) Estimation of Cu(II) using sodium thiosulphate solution (Iodometrically).
- (ii) Estimation of $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodometrically).
- (iii) Estimation of antimony in tartaremetic iodimetrically.
- (iv) Estimation of Iodine content in iodized salt.

Essential/recommended readings

Theory:

1. Lee, J. D.; (2010), **Concise Inorganic Chemistry**, Wiley India.
2. Huheey, J. E.; Keiter, E. A.; Keiter; R.L.; Medhi, O.K. (2009), **Inorganic Chemistry-Principles of Structure and Reactivity**, Pearson Education.
3. Atkins, P. W.; Overton, T. L.; Rourke, J. P.; Weller, M. T.; Armstrong, F. A. (2010), **Shriver and Atkins Inorganic Chemistry**, 5th Edition, Oxford University Press.
4. Miessler, G. L.; Fischer P. J.; Tarr, D. A. (2014), **Inorganic Chemistry**, 5th Edition, Pearson.
5. Housecraft, C. E.; Sharpe, A. G., (2018), **Inorganic Chemistry**, 5th Edition, Pearson.
6. Canham, G. R., Overton, T. (2014), **Descriptive Inorganic Chemistry**, 6th Edition, Freeman and Company.
7. Greenwood, N. N.; Earnshaw, A., (1997), **Chemistry of Elements**, 2nd Edition, Elsevier.

Practicals:

1. Jeffery, G. H.; Bassett, J.; Mendham, J.; Denney, R. C. (1989), Vogel's Text book of **Quantitative Chemical Analysis**, John Wiley and Sons.
2. Harris, D. C.; Lucy, C. A. (2016), **Quantitative Chemical Analysis**, 9th Edition, Freeman and Company.
3. Day, R. A.; Underwood, A. L. (2012), **Quantitative Analysis**, 6th Edition, PHI Learning Private Limited.

DISCIPLINE SPECIFIC CORE COURSE – 5 (DSC-5): HALOALKANES, ARENES, HALOARENES, ALCOHOLS, PHENOLS, ETHERS AND EPOXIDES

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		
Haloalkanes, Arenes,	04	02	-	02	Class 12 th with	

Haloarenes, Alcohols, Phenols, Ethers and Epoxides (DSC-5: Organic Chemistry-II)					Physics, Chemistry, Mathematics	
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Learning Objectives

The Learning Objectives of this course are as follows:

- To impart understanding of the chemistry of organic functional groups, which include haloalkanes, aromatic hydrocarbons, haloarenes and some oxygen containing functional groups, along with their reactivity patterns.
- To develop understanding of detailed reactions and mechanistic pathways for each functional group to unravel the spectrum of organic chemistry and the extent of organic transformations.
- To aid in the paramount learning of the concepts and their applications.

Learning outcomes

On completion of the course, the student will be able to:

- Explain and use reactions of arenes, haloarenes and some oxygen containing functional groups for practical applications.
- Apply the concept of protection and deprotection in organic synthesis.
- Use the synthetic chemistry learnt in this course to do functional group transformations.
- Propose plausible mechanisms for the reactions under study.

SYLLABUS OF DSC-5

Unit - 1: Haloalkanes (05 Weeks)

Alkyl halides: Methods of preparation and properties, nucleophilic substitution reactions – S_N1 , S_N2 and S_Ni mechanisms with stereochemical aspects and effect of solvent; nucleophilic substitution v/s elimination.

Organometallic compounds of Mg (Grignard reagent) – Use in synthesis of organic compounds.

Unit - 2: Aromatic Hydrocarbons (03 Weeks)

Concept of Aromaticity and anti-aromaticity; Electrophilic aromatic substitution: halogenation, nitration, sulphonation, Friedel Crafts alkylation/acylation with their mechanism. Directing effects of groups in electrophilic substitution.

Unit - 3: Aryl halides (02 Weeks)

Preparation (including preparation from diazonium salts) and properties, nucleophilic aromatic substitution; S_NAr , Benzyne mechanism. Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Unit - 4: Alcohols, Phenols, Ethers & Epoxides

(05 Weeks)

Alcohols: Relative reactivity of 1°, 2°, 3° alcohols, reactions of alcohols with sodium, HX (Lucas test), esterification, oxidation (with PCC, alkaline KMnO₄, acidic dichromate, conc. HNO₃). Oppenauer oxidation; **Diols:** oxidation of diols by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement.

Phenols: Preparation using Cumene hydroperoxide, Acidity and factors affecting it, Kolbe's–Schmidt reactions, Riemeier-Tiemann reaction, Houben–Hoesch condensation, Schotten–Baumann reaction, Fries and Claisen rearrangements and their mechanism.

Ethers and Epoxides: Acid and Base catalyzed cleavage reactions.

Practical

1. Acetylation of any one of the following compounds: amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) and phenols (β -naphthol, salicylic acid) by any one method:
 - i. Using conventional method
 - ii. Using green approach
2. 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.
3. Bromination of acetanilide/aniline/phenol by anyone of the following:
 - (a) Green method
 - (b) Conventional method
4. Nitration of nitrobenzene/chlorobenzene/phenols.
5. Haloform reaction of ethanol.
6. Oxidation of benzyl alcohol to benzoic acid
7. Estimation of the given sample of phenol/amine by:
 - a) Acetylation
 - b) Bromate-Bromide method
8. Functional group tests for alcohols, phenols, carboxylic acids, phenols, carbonyl compounds, esters.

Essential/recommended readings

Theory:

1. Morrison, R. N., Boyd, R. N., Bhattacharjee, S.K. (2010), **Organic Chemistry**, 7th Edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
2. Finar, I.L. (2002), **Organic Chemistry**, Volume 1, 6th Edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
3. Ahluwalia, V.K.; Bhagat, P.; Aggarwal, R.; Chandra, R. (2005), **Intermediate for Organic Synthesis**, I.K. International.
4. Solomons, T.W.G., Fryhle, C.B., Snyder, S.A. (2017), **Organic Chemistry**, 12th Edition, Wiley.

Practical:

1. Mann, F.G., Saunders, B.C. (2009), **Practical Organic Chemistry**, 4th Edition, Pearson Education.
2. Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (2005), **Vogel's Textbook of Practical Organic Chemistry**, Pearson.

3. Ahluwalia, V.K., Aggarwal, R. (2004), **Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis**, University Press.
4. Ahluwalia, V.K., Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
5. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi
6. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi

Suggestive readings

1. Carey, F.A., Sundberg, R. J. (2008), **Advanced Organic Chemistry: Part B: Reaction and Synthesis**, Springer.
2. Bruice, P.Y. (2020), **Organic Chemistry**, 3rd Edition, Pearson.
3. Patrick, G. (2012), **BIOS Instant Notes in Organic Chemistry**, Viva Books.
4. Parashar, R.K., Ahluwalia, V.K. (2018), **Organic Reaction Mechanism**, 4th Edition, Narosa Publishing House.

DISCIPLINE SPECIFIC CORE COURSE – 6 (DSC-6): Thermodynamics and its Applications

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		
Chemical Thermodynamics and its Applications (DSC – 6: Physical Chemistry – II)	04	03	-	01	Class XII with Physics, Chemistry and Mathematics	

Learning Objectives

The Learning Objectives of this course are as follows:

- To make students understand thermodynamic concepts, terminology, properties of thermodynamic systems, laws of thermodynamics and their correlation with other branches of physical chemistry and make them able to apply thermodynamic concepts to the system of variable compositions, equilibrium and colligative properties.

Learning outcomes

On completion of the course, the student will be able to:

- Explain and apply the three laws of thermodynamics, concept of State and Path functions, extensive and intensive properties to solve critical problems.
- Derive the expressions of ΔU , ΔH , ΔS , ΔG , ΔA for an ideal gas under different conditions and use them for solving real world problems.
- Explain the concept of partial molar properties.

SYLLABUS OF DSC-6

UNIT – 1: Basic Concepts of Chemical Thermodynamics (2 Weeks)

Intensive and extensive variables; state and path functions; isolated, closed and open systems.

Mathematical treatment - Exact and inexact differential, Partial derivatives, Euler's reciprocity rule, cyclic rule.

UNIT – 2: First law and Thermochemistry (5 Weeks)

Concept of heat, Q , work, W , internal energy, U , and statement of first law; enthalpy, H , relation between heat capacities, Joule Thompson Porous Plug experiment, Nature of Joule Thompson coefficient, calculations of Q , W , ΔU and ΔH for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions.

Enthalpy of reactions: standard states; enthalpy of neutralization, enthalpy of hydration, enthalpy of formation and enthalpy of combustion and its applications, bond dissociation energy and bond enthalpy; effect of temperature (Kirchhoff's equations) on enthalpy of reactions.

UNIT – 3: Second Law (5 Weeks)

Concept of entropy; statement of the second law of thermodynamics, Carnot cycle. Calculation of entropy change for reversible and irreversible processes (for ideal gases). Free Energy Functions: Gibbs and Helmholtz energy; variation of S , G , A with T , V , P ; Free energy change and spontaneity (for ideal gases). Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

UNIT – 4: Third Law (1 Week)

Statement of third law, unattainability of absolute zero, calculation of absolute entropy of molecules, concept of residual entropy, calculation of absolute entropy of solid, liquid and gases.

UNIT – 5: Systems of Variable Composition (2 Weeks)

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs Duhem equation, chemical potential of ideal mixtures, Change in thermodynamic functions on mixing of ideal gases.

Practical

Thermochemistry:

- (a) Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution of sulphuric acid or enthalpy of neutralization).
- (b) Determination of heat capacity of a calorimeter for different volumes using heat gained equal to heat lost by cold water and hot water.
- (c) Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- (d) Determination of the enthalpy of ionization of ethanoic acid.
- (e) Determination of integral enthalpy solution of endothermic salts.
- (f) Determination of integral enthalpy solution of exothermic salts.
- (g) Determination of basicity of a diprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
- (h) Determination of enthalpy of hydration of salt.
- (i) Study of the solubility of benzoic acid in water and determination of ΔH .

Any other experiment carried out in the class.

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 2, 6th Edition, McGraw Hill Education.
4. Kapoor, K.L., **A Textbook of Physical Chemistry**, Vol 3, 5th Edition, McGraw Hill Education.
5. McQuarrie, D. A.; Simon, J. D. (2004), **Molecular Thermodynamics**, Viva Books Pvt. Ltd.

Practical:

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

2. Kapoor, K.L. (2019), **A Textbook of Physical Chemistry**, Vol.7, 1st Edition, McGraw Hill Education.
3. 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.
2. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A.; Will, S. (2011), **Commonly asked Questions in Thermodynamics**. CRC Press.

Details of Generic Elective (GE) Courses offered by Department of Chemistry

GE COURSES –21 (4 Credits each-3T+1P/2T+2P)		
COURSE CODE	NAME OF THE COURSE	CREDITS T=Theory Credits P=Practical Credits
CHEMISTRY-GE-1	Atomic Structure and Chemical Bonding	T=2 P=2
CHEMISTRY-GE-2	Bioinorganic Chemistry	T=2 P=2
CHEMISTRY-GE-3	Basic Concepts of Organic Chemistry	T=2 P=2
CHEMISTRY-GE-4	States of Matter	T=2 P=2
CHEMISTRY-GE-5	Conductance and Electrochemistry	T=2 P=2
CHEMISTRY-GE-6	Chemistry of Food Nutrients	T=2 P=2
CHEMISTRY-GE-7	Chemistry: Statistical Methods and Data Analysis	T=2 P=2
CHEMISTRY-GE-8	Medicines in Daily Life	T=2 P=2
CHEMISTRY-GE-9	Chemistry and Society	T=2 P=2
CHEMISTRY-GE-10	Radio-chemistry in Energy, Medicine and Environment	T=3 P=1
CHEMISTRY GE-11	Chemistry in Indology and Physical & Mental Well Being	T=3 P=1
CHEMISTRY GE-12	Coordination and Organometallic Compounds	T=2 P=2
CHEMISTRY-GE-13	Chemistry of Oxygen containing Functional Groups and their Application to Biology	T=2 P=2
CHEMISTRY-GE-14	Molecules of Life	T=2 P=2

CHEMISTRY-GE-15	Chemical Kinetics and Photochemistry	T=2 P=2
CHEMISTRY-GE-16	Basics of Polymer Chemistry	T=2 P=2
CHEMISTRY-GE-17	Chemistry: Molecular Modelling, Artificial Intelligence and Machine Learning	T=2 P=2
CHEMISTRY-GE-18	Role of Metals in Medicines	T=2 P=2
CHEMISTRY-GE-19	Energy and the Environment	T=3 P=1
CHEMISTRY-GE-20	Chemistry of Fragrances and Flavours: An Industry's Perspective	T=3 P=1
CHEMISTRY-GE-21	Green Chemistry	T=2 P=2

GE Pool A: Semester I, III, V (ODD SEMESTERS)

1. GE-1: Atomic Structure and Chemical Bonding
2. GE-2: Bioinorganic Chemistry
3. GE-3: Basic Concepts of Organic Chemistry
4. GE-4: States of Matter
5. GE-5: Conductance and Electrochemistry
6. GE-6: Chemistry of Food Nutrients
7. GE- 7: Chemistry: Statistical Methods and Data Analysis
8. GE- 8: Medicines in Daily Life
9. GE- 9: Chemistry and Society
10. GE-10 Radio-chemistry in Energy, Medicine and Environment
11. GE-11: Chemistry in Indology and Physical & Mental Well Being

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

1. GE-12: Coordination and Organometallic Compounds
2. GE-13: Chemistry of Oxygen containing Functional Groups and their Application to Biology
3. GE-14: Molecules of Life
4. GE-15: Chemical Kinetics and Photochemistry
5. GE-16: Basics of Polymer Chemistry
6. GE-17: Chemistry: Molecular Modelling, Artificial Intelligence and Machine Learning
7. GE-18: Role of Metals in Medicines

8. GE-19: Energy and the Environment
9. GE-20: Chemistry of Fragrances and Flavours: An Industry's Perspective
10. GE-21: Green Chemistry

23. Ray, P. C., **A History of Hindu Chemistry: from the Earliest Times to the Middle of the Sixteenth Century A.D.**, Volume 1 – 1902, Volume 2 – 1908, The Bengal Chemical and Pharmaceutical Works Ltd
24. **“History of Chemistry in Ancient and Mideaval India”** (Edited volume of Acharya Ray’s “History of Hindu Chemistry”), Indian Chemical Society, Calcutta, 1956.
25. Harsha, N. M., Nagaraja, T. N., **The History of Hindu Chemistry**, Ancient Science of Life, 2010, 30, 58 – 61.
26. Ray, P. C., **Life and experiences of a Bengali chemist**, Two Volume Set. Calcutta: Chuckervetty, Chatterjee & Co. 1932 and 1935.
27. Ray, P. R., **Chemistry in Ancient India**, Journal of Chemical Education, 1948, 25 (6), 327.
28. Seal, B. N.(1915), **The Positive Sciences of the Ancient Hindus**, Longman Greens and Co., Kolkata.

GE 12: Chemistry: Coordination and Organometallic Compounds

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

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

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-12)	4	2		2	Class XII	

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.
- Compare synergic effect of Zeise's salt with that of carbonyls.
- Identify important structural features of tetrameric methyl lithium
- Apply 18-electron rule to rationalize the stability of metal carbonyls and related species
- Exploit IR data to explain the extent of back bonding in carbonyl complexes
- Apply 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
- Explain the meaning of the terms Δ_o , Δ_t , pairing energy, CFSE, high spin and low spin
- Explain how CFSE affects thermodynamic properties like lattice enthalpy and hydration enthalpy and use it to explain behaviour of organometallics

SYLLABUS OF GE-12

Theory:

Unit 1: Coordination Chemistry

(2 WEEKS)

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

(7 WEEKS)

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

(6 WEEKS)

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:

(15 WEEKS)

(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:

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

Practicals:

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

GE 13: Chemistry: Chemistry of Oxygen containing Functional Groups and their Applications to Biology

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
		Lecture	Tutorial	Practical/ Practice		

Chemistry of Oxygen containing Functional Groups and their Applications to Biology (GE-13)	4	2		2	Class XII	Basic knowledge of Chemistry
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Learning Objectives

The Learning Objectives of this course are as follows:

- To teach the fundamental chemistry of oxygen containing functional groups.
- To illustrate 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:

- Use reaction chemistry 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.
- Exploit the applications of functional group chemistry for biological applications.

SYLLABUS OF GE-13

Theory:

Unit 1: Alcohols (upto 5 Carbon)

(2 WEEKS)

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 KMnO₄, acidic K₂Cr₂O₇ and conc. HNO₃), Oppeneauer Oxidation, Biological oxidation Reactions

Unit 2: Phenols

(2 WEEKS)

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)

(6 WEEKS)

Reactions: Nucleophilic addition, nucleophilic addition-elimination reaction including reaction with HCN, ROH, NaHSO₃, NH₂-G derivatives. Iodoform test, Aldol condensation and its biological application, Cannizzaro's reaction, Wittig reaction, Benzoin condensation, Clemmensen reduction, Wolff Kishner reduction, Meerwein-Ponndorf Verley reduction, enzyme-catalyzed additions to α,β -unsaturated carbonyl compounds.

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

(5 WEEKS)

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:

(15 WEEKS)

(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.
3. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume II**, I K International Publishing House Pvt. Ltd., New Delhi.
4. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.

GE 14: Chemistry: Molecules of Life

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
		Lecture	Tutorial	Practical/ Practice		

Molecules of Life (GE-14)	4	2		2	Class XII	
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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:

- Demonstrate how the structure of biomolecules determines their chemical properties, reactivity and biological uses.
- Illustrate and use the knowledge gained from the mechanism of enzyme action and drug-receptor interaction for physiological purposes.
- Use the SAR studies for optimization and improvisation of biological properties of organic compounds.

SYLLABUS OF GE-14

Theory:

Unit 1: Carbohydrates

(6 WEEKS)

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

(5 WEEKS)

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

(4 WEEKS)

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, –NH₂ group, double bond and aromatic ring.

Practicals:

(15 WEEKS)

(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.
3. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume II**, I K International Publishing House Pvt. Ltd., New Delhi.
4. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.

GE 15: Chemistry: Chemical Kinetics and Photochemistry

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
		Lecture	Tutorial	Practical/ Practice		
Chemical Kinetics and Photochemistry (GE-15)	4	2		2	Class XII	

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
- To make students learn about 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:

- Explain the basic concepts of photochemistry, photochemical and photosensitized reactions and their role in biochemical systems.
- Explain the concept of rate of a reaction, order and molecularity of a reaction, various factors affecting the rate and theories of reaction rates.
- Apply the learnt concepts in studying the reaction kinetics of various reactions.

SYLLABUS OF GE-15

Theory:

Unit 1: Chemical Kinetics

(10 WEEKS)

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

(5 WEEKS)

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:

(15 WEEKS)

(Laboratory periods: 60)

1. Chemical Kinetics

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

- Acid hydrolysis of methyl acetate with hydrochloric acid.
- Compare the strength of HCl and H₂SO₄ by studying the kinetics of hydrolysis methyl acetate.
- Initial rate method: Iodide-persulphate reaction
- Integrated rate method: Saponification of ethyl acetate.
- Study the reaction 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.

GE 16: Chemistry: Basics of Polymer 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
		Lecture	Tutorial	Practical/ Practice		
Basics of Polymer Chemistry (GE-16)	4	2		2	Class XII	

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:

- Classify polymeric material.
- Illustrate different mechanisms of polymerization and polymerization techniques
- Evaluate kinetic chain length of polymers based on their mechanism
- Differentiate between polymers and copolymers
- Determine the average molecular weight of polymer using different methods.

- Differentiate between glass transition temperature (T_g) and crystalline melting point (T_m).
- Explore the polymers for useful applications in daily life.

SYLLABUS OF GE-16

Theory:

Unit 1: Introduction to polymers

(5 WEEKS)

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

(5 WEEKS)

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

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 (M_n , M_w , etc.) by end group analysis, viscometry and osmotic pressure methods. Molecular weight distribution and its significance.

Unit 3: Preparation, properties and applications

(5 WEEKS)

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:

(15 WEEKS)

(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**, Interscience (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.

GE 17: Chemistry: Molecular Modelling, Artificial Intelligence and Machine Learning

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
		Lecture	Tutorial	Practical/ Practice		
Chemistry: Molecular Modelling, Artificial Intelligence and Machine (GE-17)	4	2		2	Class XII with Physics, Chemistry, Maths/Biology	

Learning Objectives

The Learning Objectives of this course are as follows:

- To familiarize students 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 able to :

- Demonstrate reasonable proficiency in the Python Programming Language.
- Use techniques of Artificial intelligence (AI) & Machine learning (ML) for solving Chemistry based problems.

SYLLABUS OF GE-17

Theory:

Part A: Molecular Modelling

Unit 1: Introduction to computational chemistry (3 WEEKS)

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

Unit 2: Potential Energy Surfaces (2 WEEKS)

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

Unit 3: Molecular Mechanics (2 WEEKS)

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 (8 WEEKS)

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: (15 WEEKS)

(Laboratory periods: 60)

Molecular Modeling based Exercise

- 1) Write the Z-Matrix of a given set of molecules.
- 2) Carry out geometry optimisation on H₂O, H₂S, H₂Se 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 mechanical methods.

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

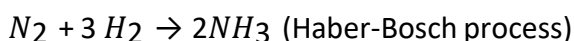
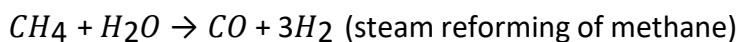
1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.

- 4) Carry out 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: (118 °C, 100 °C, 108 °C, 82 °C, 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:



- 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 and trans 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 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 academic Publisher.
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/>

GE 18: Role of Metals in Medicines

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
		Lecture	Tutorial	Practical/ Practice		
Role of Metals in Medicines (GE-18)	4	2		2	Class XII	

Learning Objectives

The Learning Objectives of this course are 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, the student will be able to :

- Explain the mode of interaction of metal ions with various biomolecules.
- Explain the role of metals in commercially available medicines.
- Explore the role of metals in diagnostics and other purposes

SYLLABUS OF GE-18

Theory:

Unit 1: Bio role of Metals

(2 WEEKS)

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

(4 WEEKS)

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

Unit 3: Metals in drugs

(3 WEEKS)

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

Unit 4: Metals in Multivitamins

(3 WEEKS)

Cyanocobalamin (Co), Ferrous fumarate (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

(3 WEEKS)

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

Practicals:

(15 WEEKS)

(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 medicines.
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

GE 19: Energy and the Environment**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
		Lecture	Tutorial	Practical/ Practice		
Energy and the Environment (GE-19)	4	3		1	Class XII	

Learning Objectives

The Learning Objectives of this course are 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, the student will be able to:

- Describe basic energy concepts
- Differentiate between 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
- Explain the importance and use of various forms of renewable energy like-Hydel, Wind, solar, etc.
- Explain the significance of environment consideration in the design, construction and operational uses

SYLLABUS OF GE-19

Theory:

Unit 1: Introduction

(4 WEEKS)

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: Energy resources 1

(4 WEEKS)

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: Energy resources 2

(4 WEEKS)

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: Pollution

(3 WEEKS)

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:

(15 WEEKS)

(Laboratory periods: 30)

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).

Practicals

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

GE 20: Chemistry of Fragrances and Flavours: An Industry's Perspective

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

	Credits	Credit distribution of the course		
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Course title & Code		Lecture	Tutorial	Practical/ Practice	Eligibility criteria	Pre-requisite of the course
Chemistry of Fragrances and Flavours: An Industry's Perspective (GE-20)	4	3		1	Class XII	

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, scents and perfumes.

Learning Outcomes

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

- Carry out synthesis of various fragrance and flavour ingredients
- Explain and use different methods for separation, purification and isolation of perfumes and flavours
- Explain how handling and other factors affect the formulation process in fragrance and flavour industry
- Uphold safety regulation and execute quality processes
- Describe the legal aspects and need for quality control in manufacturing of perfumes

SYLLABUS OF GE-20

Theory:

Unit 1: Fragrances

(6 WEEKS)

- 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

(1 WEEK)

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

Unit 3: Flavours

(6 WEEKS)

- 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

(2 WEEKS)

- 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:**(15 WEEKS)****(Laboratory Periods: 30)**

1. Extraction of D-limonene from orange peel using liquid CO₂.
2. Extraction of caffeine from coffee beans using liquid CO₂.
3. Extraction of essential oils from lemon using steam distillation
4. Extraction of essential oils from lemon using liquid CO₂.
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/>

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
		Lecture	Tutorial	Practical/ Practice		
Green Chemistry (GE-21)	4	2		2	Class XII	

Learning Objectives

The Learning objectives of this course are as follows:

- To introduce benign, sustainable and safer approach to chemistry
- To introduce the twelve principles of green chemistry and build the basic understanding of toxicity, hazard and risk assessment related to chemical substances.
- To introduce use of renewable feedstock, catalysts, alternative solvents, alternate energy sources in reaction chemistry
- To understand the green chemistry metrics and their significance

Learning Outcomes:

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

- Appreciate the success stories and real-world cases as motivation to practice green chemistry.
- Demonstrate the use of the twelve principles of green chemistry for minimizing toxicity, hazards and risks related to chemical substances.
- Design safer processes, chemicals and products through understanding of inherently safer design (ISD).
- Determine and use green chemistry matrices like atom economy, E-factor etc. to optimize organic synthesis.
- Use green chemistry in problem solving skills and critical thinking to innovate and find solutions to real world problems.

SYLLABUS OF GE-21

Theory:

Unit 1: Introduction

(4 WEEKS)

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

(6 WEEKS)

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:

(5 WEEKS)

The following Real-world Cases in green chemistry should be discussed: Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO₂ 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:

(15 WEEKS)

(Laboratory periods: 60)

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

11. Preparation and characterization of nanoparticles of gold using tea leaves/silver nanoparticles using plant extracts.
12. 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).
4. Benzoin condensation using thiamine hydrochloride as a catalyst instead of cyanide.
5. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.
6. Mechanochemical solvent free, solid-solid synthesis of azomethine using *p*-toluidine and *o*-vanillin/*p*-vanillin.
7. Microwave-assisted Knoevenagel reaction using anisaldehyde, ethylcyanoacetate and ammonium formate.
8. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
9. Photochemical conversion of dimethyl maleate to dimethyl fumarate (*cis-trans* isomerisation)
10. 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**, 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.