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DEPARTMENT OF CHEMISTRY

Semester-III

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Category-I
B Sc. (Hons) Chemistry

DISCIPLINE SPECIFIC CORE COURSE -7 (DSC-7): Chemistry of d- and f- block Elements & Quantitative Inorganic Analysis

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 d- and f- Elements & quantitative Inorganic Analysis (DSC-7)	04	02	--	02	Class 12 th with Physics, Chemistry, Mathematics	--

Learning Objectives

The Objectives of this course are as follows:

- To provide thorough knowledge about the d- and f- block elements with respect to the general group trends, physical and chemical properties of these elements.
- To familiarize the students with the d- and f-block elements and get an idea about horizontal similarity in a period in addition to vertical similarity in a group.
- To impart the knowledge about inorganic polymer
- To give an idea about the principles of gravimetric analysis.

Learning outcomes

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

- List the important properties of transition metals, lanthanoids, and actinoids
- Use Latimer diagrams to predict and identify species which are reducing, oxidizing and tend to disproportionate and calculate skip step potentials.
- Describe the classification, structure and applications of Inorganic Polymers.
- List and use the principles of gravimetric analysis for quantitative analysis

SYLLABUS OF DSC-7**UNIT – 1: Transition Elements****(12 Hours)**

General group trends with special reference to electronic configuration, colour, variable valency, magnetic properties, catalytic properties, and ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer diagrams), Frost diagrams of Mn and Cr.

A brief discussion of differences between the first, second and third transition series

UNIT – 2: Lanthanoids and Actinoids**(8 Hours)**

A brief discussion of electronic configuration, oxidation states, colour, spectral and magnetic properties. Lanthanoid contraction (causes and effects) separation of lanthanoids by ion exchange method.

UNIT – 3: Inorganic Polymer**(8 Hours)**

Comparison with organic polymers, classification, structure and applications of following inorganic polymers:

- Borates
- Silicates, silicones
- Phosphates
- Phosphazenes (for cyclic polymers, only trimer is to be discussed)

UNIT – 4: Principles of gravimetric analysis**(2 Hours)**

Particle size, Precipitation, Coagulation, Peptization, Co-precipitation, Digestion, Filtration and washing the precipitate, Drying and ignition the precipitate

Practical component**Credits: 02****(Laboratory periods:15 classes of 4 hours each)****(A) Gravimetry**

1. Estimation of Ni(II) using dimethylglyoxime (DMG).
2. Estimation of copper as CuSCN.
3. Estimation of iron as Fe₂O₃ by precipitating iron as Fe(OH)₃. (by homogeneous and heterogeneous method)
4. Estimation of Al(III) by precipitating with oxime and weighing as Al(oxime)₃ (aluminiumoxinate).

(B) Inorganic Preparations

1. Potassium aluminium sulphate $KAl(SO_4)_2 \cdot 12H_2O$ (potash alum) or Potassium chromium sulphate $KCr(SO_4)_2 \cdot 12H_2O$ (chrome alum).
2. Manganese phosphate and
3. Sodium peroxoborate

(C) Paper chromatographic separation of following metal ions (minimum two should be done):

1. Ni(II) and Co(II)
2. Cu(II) and Cd(II)
3. Fe(III) and Al(III)

Essential/recommended readings

Theory:

1. Lee, J.D.(2010), **Concise Inorganic Chemistry**, Wiley India.
2. Huheey, J.E.; Keiter, E.A.; Keiter, R.L.; Medhi, O.K.(2009), **Inorganic Chemistry- Principles of Structure and Reactivity**, Pearson Education.
3. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), **Shriver and Atkins Inorganic Chemistry**, 5th Edition, Oxford University Press.
4. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), **Inorganic Chemistry**, 5th Edition, Pearson.
5. Pfennig, B. W. (2015), **Principles of Inorganic Chemistry**. John Wiley & Sons.
6. Cotton, F.A.; Wilkinson, G. (1999), **Advanced Inorganic Chemistry**, Wiley-VCH.
7. Das, A. K.; Das, M. (2014), **Fundamental Concepts of Inorganic Chemistry**, 1st Edition, Volume 1-3, CBS Publishers & Distributors Pvt. Ltd.
8. Chandrashekar, V. (2005), **Inorganic and Organometallic Polymers**, 5th Edition, Springer Publications

Practical:

1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989), **Vogel's Textbook of Quantitative Chemical Analysis**, John Wiley and Sons,
2. Harris, D. C.; Lucy, C. A.(2016), **Quantitative Chemical Analysis**, 9th Edition, Freeman and Company.
3. Day, R. A.; Underwood, A. L. (2012), **Quantitative Analysis**, Sixth Edition, PHI Learning Private Limited.
4. Marr, G.; Rockett, B.W. (1972), **Practical Inorganic Chemistry**, Van Nostrand Reinhold.

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

DISCIPLINE SPECIFIC CORE COURSE -8 (DSC-8): Carbonyls, Carboxylic acids, Amines, Nitro compounds, Nitriles, Isonitriles and Diazonium salts

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		
Carbonyls, Carboxylic Acids, Amines, Nitro Compounds, Nitriles, Isonitriles and Diazonium salts (DSC-8)	04	03	--	01	Class 12 th with Physics, Chemistry, Mathematics	

Learning objectives

The objectives of this course are as follows:

- To infuse students with the details of the chemistry of aldehydes, ketones, carboxylic acids and their derivatives, nitro, amines and diazonium salts.
- To make students aware of the chemical synthesis, properties, reactions and key applications of the listed classes of compounds and develop understanding of detailed 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

By studying this course, students will be able to:

- Explain the chemistry of oxygen and nitrogen containing compounds.
- Use the synthetic chemistry learnt in this course to do functional group transformations.
- Propose plausible mechanisms for the reactions under study.

SYLLABUS OF DSC-8

UNIT – 1: Carbonyls, Carboxylic acid & their derivatives

(27 Hours)

Carbonyl Compounds: Reaction of carbonyl compounds with ammonia derivatives, Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α -substitution reactions, oxidations and reductions (Clemmensen, Wolff Kishner, LiAlH_4 , NaBH_4 , MPV, PDC), addition reactions of α,β -unsaturated carbonyl compounds: Michael addition.

Carboxylic acids and derivatives: Effect of substituents on acidic strength on carboxylic acids, HVZ reaction, typical reactions of dicarboxylic acids and hydroxy acids. Comparative study of nucleophilic acyl substitution for acid chlorides, anhydrides, esters and amides, Mechanism of acidic and alkaline hydrolysis of esters, Dieckmann and Reformatsky reactions, Hoffmann-bromamide degradation and Curtius rearrangement.

Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

UNIT – 2: Nitro Compounds, Amines, Diazonium salts, Nitriles and Isonitriles (18 Hours)

Nitro compounds: General methods of preparation: from alkyl halides, alkanes, oxidation of amines and oximes. Henry reaction, Nef reaction, Reduction-electrolytic reduction, reaction with nitrous acid, reduction in acidic, basic and neutral medium (for aromatic compounds)

Amines: Preparation, chirality in amines (pyramidal inversion), Basicity of amines: Effect of substituents, solvent and steric effects, distinction between Primary, secondary and tertiary amines using Hinsberg's method and nitrous acid, Gabriel Phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction and Cope elimination.

Diazonium Salts: Synthetic applications of diazonium salts including preparation of arenes, haloarenes, phenols, cyano and nitro compounds; Coupling reactions of diazonium salts (preparation of azo dyes).

Nitriles: Preparation using following reactions: Dehydration of amides and aldoximes, substitution reaction in alkyl halides and tosylates, from Grignard reagents and from dehydrogenation of primary amines. Properties: Physical properties, discussion on the following reactions with mechanism: Reaction with Grignard reagent, hydrolysis, addition reaction with HX , NH_3 , reaction with aqueous ROH , Reduction reactions-catalytic reduction and Stephen's reaction, Condensation reactions-Thorpe Nitrile Condensation.

Isonitriles: Preparation from the following reactions: Carbylamine reaction, substitution in alkyl halides and dehydrogenation of N-substituted formamides. Properties: Physical properties, discussion on the following reactions with mechanism: Hydrolysis, reduction, addition of HX , X_2 and sulphur, Grignard reaction, oxidation and rearrangement.

Practical component
(Laboratory periods:15 classes of 2 hours each)

Credits: 01

1. Preparation of oximes for aldehydes/ketones (like benzaldehyde, ethyl methyl ketone, cyclohexanone etc.)
2. Preparation of semicarbazone derivatives for aldehydes/ketones (like benzaldehyde, ethyl methyl ketone, cyclohexanone etc.)
3. Hydrolysis of amides/esters.
4. Selective reduction of *m*-dinitrobenzene to *m*-nitroaniline.
5. Preparation of S-benzylisothiuronium salts for water soluble and water insoluble carboxylic acids.
6. Systematic qualitative analysis of the given organic compounds containing monofunctional groups (aromatic hydrocarbons, alcohols, phenol) and preparation of one suitable derivative.

Students should be exposed to preparative routes for the synthesis of 3,5-dinitrobenzoate, benzoates, acetate derivatives.

Note: The above derivatives should be prepared using 0.5-1.0 g of the organic compound. The solid samples must be collected and may be used for recrystallization, melting point and compound analysis.

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. **Organic Chemistry** Volume 1, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
3. Finar, I.L. **Organic Chemistry** Volume 2, Dorling Kindersley (India) Pvt. Ltd., Pearson Education.
4. Solomons, T.W.G., Fryhle, C.B.; Snyder, S.A. (2017), **Organic Chemistry**, 12th Edition, Wiley.

Practical:

1. Vogel, A.I. (2012), **Quantitative Organic Analysis**, Part 3, Pearson Education.
2. Mann, F.G., Saunders, B.C. (2009), **Practical Organic Chemistry**, Pearson Education.
3. Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (2012), **Vogel's Textbook of Practical Organic Chemistry**, 5th Edition, Pearson.
4. Ahluwalia, V.K., Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
5. Ahluwalia, V.K., Aggarwal, R. (2004), **Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis**, University Press.

6. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi.
7. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi.

Suggestive Readings

1. Mukherji, S.M., Singh, S.P. (2017), **Reaction Mechanism in Organic Chemistry**, Trinity Press.
2. Singh, J., Awasthi, S. K., Singh, Jaya, **Fundamentals of Organic Chemistry-III**, Pragati Prakashan (2023)
3. Carey, F.A., Sundberg, R. J. (2008), **Advanced Organic Chemistry: Part B: Reaction and Synthesis**, Springer.
4. Bruice, P.Y. (2015), **Organic Chemistry**, 3rd Edition, Pearson.
5. Patrick, G. (2003), **BIOS Instant Notes in Organic Chemistry**, Viva Books.

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

DISCIPLINE SPECIFIC CORE COURSE – 9 (DSC-9): Chemical equilibrium, Ionic equilibrium, conductance and solid state

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 equilibrium, Ionic equilibrium, conductance and solid state (DSC-9)	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 the concept of chemical equilibrium and ionic equilibrium.
- To introduce the concept of electrolytes, ionization of various electrolytes, pH.
- To explain the applications of ionization in buffer, hydrolysis, acid-base titrations and indicators.
- To introduce the concept of electrolytic conductance with respect to strong and weak electrolytes and then extend it to understand concepts like ionic mobility, transference and related properties.
- To develop the advance concept of solid state with emphasis on crystal structures in general and cubic crystals in details.

Learning Outcomes:

By studying this course, students will be able to:

- Apply the concept of equilibrium to various physical and chemical processes.
- Derive and express the equilibrium constant for various reactions at equilibrium.
- Use Le Chatelier's principle to predict the thermodynamic conditions required to get maximum yield of a reaction

- Apply the concept of equilibrium to various ionic reactions.
- List different types of electrolytes and their properties related to conductance in aqueous solutions.
- Use conductance measurements for calculating many properties of the electrolytes.
- Prepare buffer solutions of appropriate pH.
- Explain the crystal properties and predict the crystal structures of cubic systems from the XRD.
- Use the instruments like pH-meter and conductivity meters.

SYLLABUS OF DSC-9

UNIT – 1: Chemical Equilibrium

(6 Hours)

Criteria of thermodynamic equilibrium, degree of advancement of reaction, Chemical equilibria in ideal gases, Thermodynamic derivation of relation between Gibbs free energy of a reaction and reaction quotient, Equilibrium constants and their dependence on temperature, pressure and concentration, Le Chatelier's Principle (Quantitative treatment), Free energy of mixing and spontaneity (qualitative discussion).

UNIT – 2: Ionic equilibrium

(12 Hours)

Strong, moderate and weak electrolytes, Arrhenius theory of electrolytic dissociation, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono and diprotic acids. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves. Theory of acid–base indicators; selection of indicators and their limitations.

UNIT – 3: Conductance

(12 Hours)

Quantitative aspects of Faraday's laws of electrolysis, Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch's law of independent migration of ions. Debye-Huckel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rule. Ionic velocity, mobility and their determination, transference number and its relation to ionic mobility, determination of transference number using Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations (v) hydrolysis constants of salts.

UNIT – 4: Solid state

(15 Hours)

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary idea of symmetry, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl.

Practical component

Credit:01

(Laboratory periods: 15 classes of 2 hours each)

pH metry:

1. Study the effect of addition of HCl/NaOH on pH to the solutions of acetic acid, sodium acetate and their mixtures.
2. Preparation of buffer solutions of different pH values
 - a. Sodium acetate-acetic acid
 - b. Ammonium chloride-ammonium hydroxide
3. pH metric titration of
 - a. Strong acid with strong base
 - b. Weak acid with strong base. Determination of dissociation constant of a weak acid.

Conductometry:

1. Determination of cell constant
2. Determination of conductivity, molar conductivity, degree of dissociation and dissociation constant of a weak acid.
3. Perform the following conductometric titrations:
 - a. Strong acid vs. strong base
 - b. Weak acid vs. strong base
 - c. Mixture of strong acid and weak acid vs. strong base
 - d. Strong acid vs. weak base

p-XRD (*p-XRD crystal pattern to be provided to the students*)

1. Differentiate and classify the given set of the diffraction pattern as crystalline materials or amorphous (Glass) substance.
2. Carry out analysis of a given set of p-XRD and determine the type of the cubic crystal structure
 - a. NaCl
 - b. CsCl
 - c. KCl
3. Determination of approximate crystal size from a given set of p-XRD

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. McQuarrie, D. A.; Simon, J. D. (2004), **Molecular Thermodynamics**, Viva Books Pvt. Ltd.
5. Kapoor, K.L. (2015), **A Textbook of Physical Chemistry**, Vol 1, 6th Edition, McGraw Hill Education.

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.

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POOL OF DISCIPLINE SPECIFIC ELECTIVE COURSE

DISCIPLINE SPECIFIC ELECTIVE COURSE -1 (DSE-1): Nuclear and Environmental Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

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

Learning Objectives

The Objectives of this course are as follows:

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

Learning outcomes

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

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

SYLLABUS OF DSE-1

Unit-1 : Nuclear Chemistry

(21 Hours)

The nucleus: subatomic particles, e liquid drop model; forces in nucleus-mesons; stability of nucleus-n/p ratio, binding energy; radioactive elements.

Radioactive decay- α -decay, β -decay, γ -decay; neutron emission, positron emission; unit of radioactivity (curie); half life period; radioactive displacement law, radioactive series.

Measurement of radioactivity: ionization chamber, Geiger Counters, Scintillation counters.

Nuclear reactions: Nuclear fission-theory of nuclear fission; chain reaction; nuclear fusion; nuclear reactors-fast breeder reactors, fuels used in nuclear reactors, separation of isotopes, moderators, coolants; nuclear reactors in India.

Applications: Dating of rocks and minerals, carbon dating, neutron activation analysis, isotopic labeling studies, nuclear medicine- ^{99m}Tc radio pharmaceuticals.

Nuclear disasters – Chernobyl disaster, Three Mile Island Disaster, Disposal of nuclear waste and its management.

UNIT – 2: Air Pollution

(12 Hours)

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

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

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

UNIT – 3 : Water Pollution:

(12 Hours)

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

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

Practical component

Credits: 01

(Laboratory periods:15 classes of 2 hours each)

(At least four experiments to be performed)

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

Essential/recommended readings

Theory:

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

Practical:

1. Vowles, P.D.; Connell, D.W. (1980), **Experiments in Environmental Chemistry: A Laboratory Manual**, Vol.4, Pergamon Series in Environmental Science.

2. Gopalan, R.; Anand, A.; Sugumar R.W. (2008), **A Laboratory Manual for Environmental Chemistry**, I. K. International.

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

DISCIPLINE SPECIFIC ELECTIVE COURSE - 2 (DSE-2): Inorganic materials of industrial importance

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Inorganic Materials of Industrial Importance (DSE-2)	04	03	--	01	Class 12 th with Physics, Chemistry	--

Learning Objectives

The objectives of this course are as follows:

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

Learning outcomes

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

- State the composition and applications of the different kinds of glass.
- State the composition of cement and discuss the mechanism of setting of cement.
- Defend the suitability of fertilizers for different kinds of crops and soil.

- Explain the process of formulation of paints and the basic principle behind the protection offered by the surface coatings.
- Describe the principle, working and applications of different batteries.
- Evaluate the synthesis and properties of nano-dimensional materials, various semiconductor and superconductor oxides.

SYLLABUS OF DSE-2

Unit 1: Silicate Industries

(6 Hours)

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

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

Unit 2: Fertilizers

(6 Hours)

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

Unit 3: Surface Coatings

(18 Hours)

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

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

Unit 4: Batteries

(3 Weeks)

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

Unit 5: Nano dimensional materials

(2 Weeks)

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

Practical component

Credits: 01

(Laboratory periods:15 classes of 2 hours each)

(At least four experiments to be performed)

1. Detection of constituents of Ammonium Sulphate fertilizer (Ammonium and Sulphate ions) by qualitative analysis and determine its free acidity.
2. Detection of constituents of CAN fertilizer (Calcium, Ammonium and Nitrate ions) fertilizer and estimation of Calcium content.
3. Detection of constituents of Superphosphate fertilizer (Calcium and Phosphate ions) and estimation of phosphoric acid content.
4. Analysis of (Cu, Ni) in alloy or synthetic samples (methods involving Gravimetry and Spectrophotometry).
5. Analysis of (Cu, Zn) in alloy or synthetic samples (Multiple methods involving Iodometry, and Potentiometry).
6. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.
7. Synthesis of silver nanoparticles by green and chemical approach methods and its characterization using UV-visible spectrophotometer

Essential/recommended readings

Theory:

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

Practical:

1. Svehla, G.(1996),**Vogel's Qualitative Inorganic Analysis**, Prentice Hall.

- Banewicz, J. J.; Kenner, C.T. **Determination of Calcium and Magnesium in Limestones and Dolomites**, Anal. Chem., 1952, 24 (7), 1186–1187.
- Ghorbani, H. R.; Mehr, F.P.; Pazoki, H.; Rahmani B. M. **Synthesis of ZnO Nanoparticles by Precipitation Method**. Orient J Chem 2015;31(2).
- Orbaek, W.; McHale, M.M.; Barron, A.R. **Synthesis and characterization of silver nanoparticles for an undergraduate laboratory**, J. Chem. Educ. 2015, 92, 339–344.

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

DISCIPLINE SPECIFIC ELECTIVE COURSE – 3 (DSE-3): Green Chemistry in Organic Synthesis

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Green Chemistry in Organic Synthesis (DSE-3)	04	03	--	01	Class 12 th with Physics, Chemistry	Basic knowledge of organic reactions

Learning objectives

The objectives of this course are as follows:

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

develop and run chemical processes in a sustainable way.

Learning outcomes

By studying this course, students will be able to:

- List the twelve principles of green chemistry and build the basic understanding of toxicity, hazard and risk related to chemical substances.
- Calculate atom economy, E-factor and relate them in all organic synthesis
- State the uses of catalyst over stoichiometric reagents
- Debate and use green solvents, renewable feedstock, and renewable energy sources for carrying out safer chemistry
- Use green chemistry for problem solving, innovation and finding solutions to environmental problems.
- Design safer processes, chemicals, and products through understanding of inherently safer design (ISD)
- Discuss the success stories and use real-world cases to practice green chemistry

SYLLABUS OF DSE-3

UNIT – 1: Introduction

(3 Hours)

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

UNIT – 2: Application of Green Chemistry Principles

(36 Hours)

Principles of Green Chemistry and designing a chemical synthesis

Concept familiarization and application of green chemistry principles using specific examples

1. Prevention of waste/ by products; waste or pollution prevention hierarchy
2. Green metrics to assess greenness of a reaction: Calculation of atom economy of the rearrangement, addition, substitution, and elimination reactions; calculation of E-factor for industrial processes
3. Prevention/ minimization of hazardous/ toxic products
4. Safer Solvent and Auxiliaries: Problems associated with conventional reaction media Some Common Green solvents: Introduction, application, advantages, and disadvantages of green solvents in organic synthesis (taking suitable examples). Special emphasis on the following:
 - i. Super Critical Fluids (with special reference to carbon dioxide)
 - ii. Water: Concept of In-water, and on-water reactions (with special reference to synthesis of terpinol and linalool in water, Benzoin condensation, Heck reaction)
 - iii. Ionic Liquids: Physical properties and classification of Ionic Liquids (with special reference to Diels Alder reaction and Coumarin synthesis in ionic liquids)

- iv. Biomass derived Solvents: Physicochemical properties, Use of glycerol and its derivatives (Mizoroki–Heck reaction) and 2-methyltetrahydrofuran (Suzuki–Miyaura reaction).
5. Design for energy efficiency: Phenomenon of accelerating organic reactions by using the following Green Chemistry tools (taking suitable examples) and its advantages:
 - i. Mechanochemistry
 - ii. Ultrasound assisted reactions: Taking examples like Simmons Smith reaction, Diels–Alder reaction,
 - iii. Microwave assisted reactions: Special emphasis on solvent-free synthesis- copper phthalocyanine and aspirin, In-water reactions-Hofmann Elimination, methyl benzoate to benzoic acid and Decarboxylation reaction;
 - iv. Electrocatalysis: Taking examples like adiponitrile synthesis, synthesis of 3-bromothiophene.
 - v. Visible light induced Reactions: with examples such as, syntheses of caprolactam and vitamin D₃, cis-trans isomerization of alkenes
6. Use of renewable starting materials: Illustrate with few examples such as biodiesel, bioethanol, polymers from renewable resources (PLA from corn), Synthesis and properties of 2-Methyltetrahydrofuran, furfural and 5-Aminolevulinic acid (DALA) from levulinic acid
7. Avoidance of unnecessary derivatization – careful use of blocking/protecting groups (taking specific examples like selective oxidation of aldehydic group and synthesis of 6-Aminopenicillanic Acid (6-APA) from penicillin G
8. Catalysis and green chemistry
Introduction to Catalysis (including concept of selectivity, turnover frequency and turnover number), Types of Catalysts: Heterogeneous catalysis and homogeneous catalysis (H-beta and zeolites in organic synthesis), General catalytic cycle for heterogeneous catalysis; Asymmetric catalysis (Monsanto route to L-dopa via asymmetric hydrogenation, synthesis of carbapenem via Asymmetric reduction); Photocatalysis (with special reference to TiO₂); Biocatalysis (Synthesis of adipic acid/catechol using biocatalyst) and Nanocatalysis (oxazole synthesis using nanocatalyst)
9. Design for degradation: (Illustrate with the help of examples: soaps and detergents, pesticides, polymers)
10. Real Time monitoring of chemical processes using inline, offline, and online techniques
11. Inherently safer design/chemistry:
Principle and subdivision of ISD, Bhopal Gas Tragedy (safer route to carbaryl) and Flixborough accident (safer route to cyclohexanol, Asahi Process)

UNIT – 3: Industrial Applications and Success Stories

(6 Hours)

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

Practical component

Credits: 01

(Laboratory periods:15 classes of 2 hours each)

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

1. Preparation and characterization of nanoparticles of gold using tea leaves/silver nanoparticles using plant extracts.
2. Preparation of biodiesel from waste cooking oil and characterization (TLC, pH, solubility, combustion test, density, viscosity, gel formation at low temperature and IR can be provided).
3. Benzoin condensation using thiamine hydrochloride as a catalyst instead of cyanide.
4. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.
5. Mechanochemical solvent free, solid-solid synthesis of azomethine using p-toluidine and o-vanillin/p-vanillin.
6. Microwave-assisted Knoevenagel reaction using anisaldehyde, ethylcyanoacetate and ammonium formate.
7. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
8. Photochemical conversion of dimethyl maleate to dimethyl fumarate (cis-trans isomerisation)
9. Benzil- Benzilic acid rearrangement: Preparation of benzilic acid in solid state under solvent-free condition.
10. Preparation of dibenzalacetone by cross aldol condensation reaction using base catalysed green method.

Essential/recommended readings

Theory:

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

Practicals:

1. Kirchoff, M.; Ryan, M.A. (2002), **Greener approaches to undergraduate chemistry experiment**, American Chemical Society, Washington DC.

- Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K. (2013), **Green Chemistry Experiments: A monograph**, I.K. International Publishing House Pvt Ltd. New Delhi.
- 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.
- 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.
- Sidhwani, I.T; Sharma, R.K. (2020), **An Introductory Text on Green Chemistry**, Wiley India Pvt Ltd.
- Monograph on Green Chemistry Laboratory Experiments**, Green Chemistry Task Force Committee, Department of Science and Technology, Government of India.
- Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–I**, I K International Publishing house Pvt. Ltd, New Delhi
- Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume–II**, I K International Publishing house Pvt. Ltd, New Delhi

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

DISCIPLINE SPECIFIC ELECTIVE COURSE – 4 (DSE-4): Reactions, Reagents and Chemical Process

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Reactions, Reagents and Chemical Process (DSE-4)	04	03	--	01	Class 12 th with Physics, Chemistry	Basic knowledge of organic reactions

Learning objectives

The objectives of this course are as follows:

- To study the important organic name and rearrangement reactions that are crucial for the synthesis of valuable organic compounds.
- To give the knowledge belonging to the role of reagents in organic reactions for the synthesis of chemo-, diastereo- and enantio-selective products.

- To impart the knowledge of process chemistry that is a key part of the large-scale synthesis of chemical products essential for day-to-day life

Learning outcomes

By studying this course, students will be able to:

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

SYLLABUS OF DSE-4

UNIT – 1: Name Reactions

(15 Hours)

Application, scope and mechanism of following reactions: Prevost Reaction, Chugaev Reaction, Maukaiyama Aldol Reaction, Mzingo Reaction, Ramberg Backlund Reaction, Shapiro Reaction, Barbier Reaction, Clark- Eschweiler Reaction, Darzen's Reaction, Julia-Olifination Reaction, Tiffeneaus Damjanov Reaction, Darkin West Reaction, Bischler-Napieralaski Reaction, Birch reduction of aromatic compounds, Appel Reaction, Mitsunobu Reaction, Corey Kim Oxidation, Azide-alkyne 1,3-dipolar cycloaddition reaction, Olefin metathesis: Grubbs reaction, Heck Reaction, Suzuki coupling and Wittig reaction.

UNIT – 2: Reducing Reagents

(9 Hours)

Reactions, mechanism and applications of following reducing agents: Sodium borohydride, Lithium aluminium hydride, NaBH_3CN , DIBALH, lithium-tri-*tert*-butoxyaluminum hydride, Red-Al $\text{Na}[\text{AlH}_2(\text{OCH}_2\text{OCH}_2\text{OCH}_3)_2]$, Zinc borohydride, L and K selectrides, LiBHEt_3 and KBHEt_3 , Luche Reagent $\text{NaBH}_4\text{-CeCl}_3$, $\text{K}[\text{BH}(\text{OAc})_3]$, *bis*-Boric Acid (BBA), Catecholborane, DEMS (Diethoxymethylsilane), 3-Mercapto propionic acid, Polymethylhydrosiloxane (PMHS), Schwartz's Reagent (Zirconocene chloride hydride).

UNIT – 3: Oxidizing Reagents

(9 Hours)

Reactions, mechanism and applications of following oxidizing agents: Jones Reagent (CrO_3 , H_2SO_4 , H_2O), Swern Reagent (DMSO, oxalyl chloride), Dess Martin, TEMPO, TPAP (Tetrapropyl ammonium perruthenate), Fetizon's Reagent, Fenton's Reagent [H_2O_2 + Fe(II) ion], Sodium perborate NaH_2BO_4 , Sodium Bismuthate NaBiO_3 , ABNO (9-Azabicyclo[3.3.1]nonane N-oxyl), DEAP (Diethyl allyl phosphate, $\text{CH}_2=\text{CH}-\text{CH}_2-\text{OPO}(\text{OEt})_2$), AZADO (2-Azaadamantane N-oxyl), Wacker oxidation.

UNIT – 4: Process Chemistry

(12 Hours)

1. Process chemistry a) Introduction, stages of scale up process: Bench, pilot, and large-scale process with at least two examples of scale up process of API. b) In-process control and validation of large-scale process.
2. Unit Processes: The following unit processes should be studied with mechanism and one example of each process Nitration: Nitrating agents, process equipment for technical nitration. Halogenation: Types of halogenations, catalytic halogenations. Reduction: Catalytic hydrogenation, hydrogen transfer reactions, metal hydrides. Oxidation: Types of oxidative reactions, and non-metallic oxidizing agents such as H₂, sodium hypochlorite, oxygen gas, ozonolysis.

Practical component

Credits: 01

(Laboratory periods:15 classes of 2 hours each)

1. Oxidation of alcohols to acid using Jones reagent.
2. Reduction of acetophenone and its derivatives to 1-phenyl ethanol derivatives by NaBH₄.
3. Reduction of 4-tert-butyl-cyclohexanone to cis and trans 4-tert-butyl-cyclohexanol.
4. Synthesis of 2,5-dimethyl-2,5-hexanediol from tert-butanol using Fenton's reagents.
5. Wittig reaction of benzyltriphenylphosphonium chloride and 4-bromobenzaldehyde using potassium phosphate (tribasic).
6. Substitution (S_N2) reaction of 1-iodobutane and 2-naphthol.
7. Aldol condensation reaction: solventless synthesis of chalcones.
9. Borohydride reduction of a ketone: hydrobenzoin from benzil.
10. Visit to chemical industry for the demonstration of pilot scale.

Essential/recommended readings

Theory:

1. Clayden, J. Greeves, N., Warren, S. **Organic Chemistry**, South Asian Edition, Oxford University Press, USA
2. Gadamasetti K., **Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever- Changing Climate-An Overview**, Vol-2, CRC Press, London.
3. Murphy R.M., **Introduction to Chemical Processes: Principles, Analysis, Synthesis**, McGraw-Hill Education, New York.
4. Harrington P. J., **Pharmaceutical Process Chemistry for Synthesis: Rethinking the Routes to Scale up**, John Wiley and Sons, Inc, New Jersey.
5. Parashar, R.K.; Ahluwalia, V.K. (2018), **Organic Reaction Mechanism**, 4th Edition, Narosa Publishing House.
6. Singh J., S. K. Awasthi, Singh Jaya (2023) **Fundamental of Organic Chemistry**, Paper III, Pragati Prakashan.

Practical:

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

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

DISCIPLINE SPECIFIC ELECTIVE COURSE -5(DSE-5): Solutions, Colligative properties, Phase Equilibria and adsorption

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Solutions, Colligative properties, Phase Equilibria and adsorption (DSE-5)	04	03	-	01	Class 12 th with Physics, Chemistry	

Learning Objectives

The Learning Objectives of this course are as follows:

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

Learning outcomes

By studying this course, students will be able to:

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

SYLLABUS OF DSE-5

UNIT-1: Solutions and Colligative Properties

(12 Hours)

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

UNIT-2: Phase Equilibria

(24 Hours)

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

Three component systems, water-chloroform-acetic acid system, triangular plots.

UNIT-3: Surface chemistry

(9 Hours)

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

Practical component

(Laboratory periods: 15 classes of 2 hours each)

Credit: 01

Practical

Phase Equilibrium

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

Adsorption

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

Essential/recommended readings

Theory:

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

Practical:

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

Suggestive readings

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

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

DISCIPLINE SPECIFIC ELECTIVE COURSE- 6 (DSE-6): Applications of computers in Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

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

Learning Objectives

The Learning Objectives of this course are as follows:

To make the students learn the working of computer and its applications in chemistry *via* programming language, C language and use of software as a tool to understand chemistry and solve chemistry-based problems.

Learning outcomes

By studying this course, students will be able to:

- Use commands and library functions in programming in C language.
- Develop algorithm to solve problems and write corresponding programs in C language for performing calculations involved in laboratory experiments.
- Use various spreadsheet software to perform theoretical calculations and plot graphs

SYLLABUS OF DSE-6

UNIT 1: Introduction to Basic Computer System

(6 Hours)

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

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

UNIT 2: Commands and Library functions in C language

(18 Hours)

C language for solving some of the basic and complicated chemistry problems). QB4 version of C language can be used.

Numeric constants, variables & its declaration, Arithmetic expressions, hierarchy of operations, inbuilt functions and header files. Syntax and use of the following commands in C language: scanf, printf, fscanf and fprintf; goto, relational operators, *if-else* statement; *while*, *for* and *do while* loops, *switch-break* statements; header files (<stdio.h>, <stdlib.h>, <math.h>, <ctype.h>, <malloc.h>, <string.h>), arrays & pointers, library functions (abs & fabs, int, float, double, ceil, char, exp, log, rand, sqrt, \t, \v, \n and trigonometric Functions), defining and accessing functions, gnuplot- syntax and commands

Simple programs using C commands, Matrix addition and multiplication

UNIT 3: Use of C language for solving problems in Chemistry

(21 Hours)

Solution of quadratic equation, polynomial equations (formula, iteration, Newton – Raphson methods and binary bisection) with examples of polynomial equations used in chemistry; Numerical differential, Numerical integration (Trapezoidal and Simpson's rule), Calculation of area under the curves for chemistry problems, e.g., entropy calculations, Simultaneous equations, Statistical analysis-mean, variance, standard deviation, error, least square method.

Plotting linear graphs using experimental data, plotting (i)trigonometric functions-particle in a one-dimensional box(ii) exponential function (iii) Ideal gas isotherms. Plotting van der Waals Isotherms, and observe whether van der Waal gas equation is valid at temperatures lower than critical temperature where we require to solve a cubic equation.

Practical Component

Credit: 01

(Laboratory periods: 15 classes of 2 hours each)

Computer programs using C language based on numerical methods

1. Simple programs to calculate numerical values of chemistry problems.
2. Roots of equations: (e.g. volume of gas using Van der Waals equation and comparison with ideal gas, pH of a weak acid).
3. Solving polynomial equation using iterative method. (Van der Waal's equation of state, pH of a weak acid using exact expression)

4. Solving polynomial equation using Newton-Raphson's method. (Van der Waal's equation of state, pH of a weak acid using exact expression)
5. Matrix operations: addition, multiplication and transpose
6. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
7. Numerical integration using trapezoidal method. (e.g. entropy/ enthalpy change from heat capacity data).
8. Numerical integration using Simpson's rule
9. Mean, standard deviation
10. Least square curve fitting method for linear equation.
11. Calculate the relative intensities of peaks of a proton obtained after spin-spin coupling with 4 equivalent neighbouring protons in a high-resolution NMR spectrum using GOSUB RETURN.

Computer programs using C language for plotting graphs

1. Van der Waals isotherm
2. Compressibility versus pressure curves
3. Maxwell distribution curves
4. Concentration-time graph using kinetics data
5. pH metric titration curve
6. Conductometric titration curves for strong acid-strong base titrations.
7. Calibration curve using Lambert Beer's law
8. Particle in a one-dimensional box.

Note: Minimum 12 exercises is to be performed relating to C language

Plotting graphs using spreadsheet

1. Particle in a one-dimensional box.
2. van der Waals isotherms below critical temperature, at critical temperature and above critical temperature.
3. Radial plots and radial distribution functions for orbitals of hydrogen atom.
4. Plotting characteristics graphs of zero, first and second order reactions using concentration time data and determine the order of the reaction.

Essential/recommended readings

Theory:

1. McQuarrie, D. A. (2008), **Mathematics for Physical Chemistry**, University Science Books.

2. Mortimer, R. (2005), **Mathematics for Physical Chemistry**, 3rd Edition, Elsevier.
3. Steiner, E. (1996), **The Chemical Maths Book**, Oxford University Press.
4. Yates, P. (2007), **Chemical Calculations**, CRC Press.
5. Harris, D. C. (2007), **Quantitative Chemical Analysis**, 6th Edition, Freeman, Chapters 3-5.
6. Rajaraman, V., **Computer Programming in C**, PHI Learning Private Limited.
7. Gottfried, B., **Programming with C**, Tata McGraw Hills Education Pvt. Ltd., 3rd Edition.

Practical:

1. Levie, R.D. (2001), **How to use Excel in analytical chemistry and in general scientific data analysis**, Cambridge University Press.
2. Kapoor, K.L. (2019), **A Textbook of Physical Chemistry**, Vol.7, 1st Edition, McGraw Hill Education.

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