Introduction, classification, uses, aromaticity of polynuclear compounds, Structure elucidation of naphthalene, preparation and properties of naphthalene and anthracene.

UNIT-2: Pharmaceutical Compounds (12 Hours)

Introduction, classification, general mode of action of antipyretics and analgesics, aspirin; Synthesis, uses and side effects of the following drugs:
Antipyretics - Paracetamol (with synthesis and mode of action); Analgesics- Ibuprofen (with synthesis and overview of the mode of action); Antimalarials - Chloroquine (synthesis and mode of action).
An elementary treatment of Antibiotics and detailed study of chloramphenicol including mode of action. Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine)**.**

UNIT-3: UV-Visible and IR Spectroscopy (12 Hours)

UV-Visible and IR Spectroscopy and their application to simple organic molecules. Electromagnetic radiations and their properties; double bond equivalence and hydrogen deficiency. UV-Visible spectroscopy (electronic spectroscopy): General electronic transitions, λ_{max} & ε_{max}, chromophores &auxochromes, bathochromic & hypsochromic shifts. Application of Woodward rules for the calculation of λ_{max} for the following systems: conjugated dienes - alicyclic, homoannular and heteroannular; α, β-unsaturated aldehydes and ketones, charge transfer complex.

Infrared (IR) Spectroscopy: Infrared radiation and types of molecular vibrations, the significance of functional group & fingerprint region. IR spectra of alkanes, alkenes, aromatic hydrocarbons (effect of conjugation and resonance on IR absorptions), simple alcohols (inter and intramolecular hydrogen bonding and IR absorptions), phenol, carbonyl compounds, carboxylic acids and their derivatives (effect of substitution on >C=O stretching absorptions).

Practical component Credit:02

(Laboratory periods: 15 classes of 4 hours each)

1. Isolation and estimation of the amount of aspirin in a commercial tablet.
2. Preparation of Aspirin.
3. Synthesis of ibuprofen.
4. Systematic qualitative identification and derivative preparation of organic compounds (Aromatic hydrocarbons, Aryl halides)
5. Detection of simple functional groups through examination of IR spectra (spectra to be provided). IR spectra of simple compounds like phenols, aldehydes, ketones, carboxylic acids may be given.
6. Differentiation between of o-/p-hydroxybenzaldehyde by IR spectroscopy (Spectra to be provided).
7. Differentiation between benzoic acid and cinnamic acid by UV spectroscopy.
8. Diel's Alder reaction using Anthracene and Maleic anhydride.
9. Partial Reduction of m-dinitrobenzene to m-nitroaniline and then analysing the IR spectra of reactant and Product.
10. Laboratory preparation of Paraacetamol.

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. **Organic Chemistry,** Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Bahl, A; Bahl, B. S. (2012), **Advanced Organic Chemistry**, S. Chand.
4. Pavia, D.L. **Introduction to Spectroscopy**, Cengage learning (India) Pvt. Ltd.
2. Kemp, W. (1991), **Organic Spectroscopy**, Palgrave Macmillan.

Practicals:

1. Ahluwalia, V.K.; Dhingra, S.; Gulati, A. (2005), **College Practical Chemistry,** University Press (India) Ltd.
2. Ahluwalia, V.K.; Dhingra, S. (2004), **Comprehensive Practical Organic Chemistry: Qualitative Analysis**, University Press.
3. Vogel, A.I. (1972), **Textbook of Practical Organic Chemistry**, Prentice-Hall.
4. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.
5. Pasricha, S., Chaudhary, A. (2021), **Practical Organic Chemistry: Volume I**, I K International Publishing House Pvt. Ltd., New Delhi.

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DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE 3:

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		
Chem-DSE 3: Computer Applications in Chemistry	**04**	**02**	**-**	**02**	**Class XII with Science**	

Learning Objectives

The Learning Objectives of this course are as follows:

- To introduce the students to basic computer skills that will help them in solving chemistry problems using spreadsheets and BASIC language.
- To acquaint the students with different software for data tabulation, calculation, graph plotting, data analysis and document preparation.
- To expose the students to the concept of molecular modelling, its applications to various molecular systems, energy minimization techniques, analysis of Mulliken Charge and ESP Plots.

Learning outcomes

By studying this course, students will be able to:

- Have knowledge of most commonly used commands and library functions used 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 CHEM-DSE-3

UNIT-1: Programming using BASIC **(20 Hours)**

Programming Language – Elements of BASIC language, Numeric and string Constants and Variables, arithmetic expressions, hierarchy of operations, inbuilt functions. Syntax and use of the various QBASIC commands: REM, CLS, INPUT, PRINT, GOTO, IF, IF…THEN, IF..THEN..ELSE, IF and END IF, FOR and NEXT etc., DIM, READ, DATA, GOSUB,

RETURN, RESTORE, DEF FNR and Library Functions, Simple programs based on usage of the commands mentioned above.

Statistical analysis using BASIC: Mean, Least square fit - Linear regression, variance, standard deviation.

UNIT-2: Handling of Numerical Data (4 Hours)

Spreadsheet software: MS Excel. Creating a spreadsheet, entering and formatting information, applying basic functions and formulae to the data, drawing charts, tables and graphs, displaying the equation of graph along with the R^2 value, incorporating tables and graphs in Word files, graphical solution of equations, plotting pressure-volume curves of van der Waals gases, Maxwell-Boltzmann distribution, concentration versus time graphs, spectral data, titration curves, etc.

UNIT-3: Molecular Modelling (6 Hours)

Introduction to molecular modelling, overview of classical and quantum mechanical methods (molecular mechanics, semi empirical, ab initio and DFT), general considerations and comparison of these methods.

Practical component Credit:02

(Laboratory periods: 15 classes of 4 hours each)

Exercises of Programing

1. Calculate pressure of a real gas using Van der Waal's Equation.
2. Calculate the most probable speed, average speed and root men square velocity of an ideal gas.
3. Roots of quadratic equations
4. Binomial coefficient using GOSUB statement.
5. Mean, standard deviation
6. Least square curve fitting method for linear equation.

Plotting graphs using a spreadsheet

1. van der Waals isotherms
2. Maxwell-Boltzmann distribution curves as function of temperature and molecular weight
3. Plot the conductometric titration curve for

   a) strong acid vs strong base and b) weak acid vs strong base
4. Plot the pH metric titration curve for

   a) strong acid vs strong base and b) weak acid vs strong base and determine the pK_a of the weak acid
5. Plot the graphs for the kinetics of first order reaction and determine the rate constant
6. Plot the UV-vis absorbance spectra and determine the molar absorption coefficient.

Molecular Modelling

1. Optimize and compare the geometry parameters of H_2O and H_2S using Argus Lab.
2. Compare the basicities of N atom in ammonia, methylamine, dimethylamine and trimethylamine using Argus Lab by comparing Mulliken charges and ESP map in Argus Lab.
3. Compare C-C bond lengths and bond order in ethane, ethene and ethyne using Argus Lab.
4. Determine enthalpy of isomerization of cis and trans-2-butene in Argus Lab.
5. Compare the HAH bond angles for the second row hydrides (BeH_2, CH_4, NH_3, H_2O) and compare with the results from qualitative MO theory.

References:

Theory:

1. Levie, R. de. (2001), **How to use Excel in analytical chemistry and in general scientific data analysis**, Cambridge Univ. Press.
2. Venit, S.M. (1996),**Programming in BASIC: Problem solving with structure and style**. Jaico Publishing House.
3. Lewars, E. (2003), **Computational Chemistry,** Kluwer academic Publisher.
4. Cramer, C.J.(2004), **Essentials of Computational Chemistry,** John Wiley & Sons.
5. Hinchcliffe, A. (1996), **Modelling Molecular Structures,** John Wiley & Sons.
6. Leach, A.R.(2001), **Molecular Modelling,** Prentice-Hall.

Practicals:

1. Lewars, E. **(2003), Computational Chemistry,** Kluwer academic Publisher.
2. Cramer, C.J. **(2004), Essentials of Computational Chemistry,** John Wiley & Sons.
3. Hinchcliffe, A. **(1996), Modelling Molecular Structures,** John Wiley & Sons.

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