Annexure-4.01.50(ii)
Item No. 4-1-50

INDEX

DEPARTMENT OF CHEMISTRY

Semester-III

Bachelor of Sciences (Life Sciences/ Physical Sciences)

Category II

BSc (Life Sciences/ Physical Sciences) with Chemistry as one of the Core Discipline

DISCIPLINE SPECIFIC CORE COURSE -7: Chemistry -III Chemical Energetics and Equilibria

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 Energetics and Equilibria (DSC-7: Chemistry 03:	04	02	--	02	Class 12th with Physics, Chemistry, Mathematics	NA

Learning objectives

The objectives of this course are as follows:

- To develop basic understanding of the chemical energetics, laws of thermodynamics and ionic equilibrium.
- to provides basic understanding of the behaviour of electrolytes and their solutions.
- To make students learn about the properties of ideal and real gases and deviation from ideal behavior

Learning outcomes

By studying this course, students will be able to:

- Explain the laws of thermodynamics, thermochemistry and equilibria.
- Use the concept of pH and its effect on the various physical and chemical properties of the compounds.
- Use the concepts learnt to predict feasibility of chemical reactions and to study the behaviour of reactions in equilibrium

SYLLABUS

UNIT-1: Chemical Energetics **(16 Hours)**

Recapitulation of Intensive and extensive variables; state and path functions; Isolated, closed and open systems

First law

Concept of heat (Q), work (W), internal energy (U), and statement of first law; enthalpy (H), relation between heat capacities for ideal gas, Joule's experiment, calculations of Q, W, ΔU and ΔH for reversible expansion of ideal gases under isothermal conditions.

Thermochemistry

Enthalpy of reactions: standard states; enthalpy of neutralization, enthalpy of ionization enthalpy of hydration, enthalpy of formation and enthalpy of combustion, Integral enthalpy of solution, bond dissociation energy and bond enthalpy; Hess's law, Born Haber's cycle (NaCl/ KCl).

Second Law

Concept of entropy; statements of the second law of thermodynamics (Kelvin and Clausius). Calculation of entropy change for reversible processes (for ideal gases). Free Energy Functions: Gibbs and Helmholtz energy (Non-PV work and the work function); Free energy change and concept of spontaneity (for ideal gases).

Third Law

Statement of third law, qualitative treatment of absolute entropy of molecules (examples of NO, CO), concept of residual entropy

UNIT-2: Chemical Equilibrium **(4 Hours)**

Criteria of thermodynamic equilibrium. Free energy change in a chemical reaction and equilibrium constant, exergenic and endergenic reactions with examples such conversion of ATP to ADP or vice verca,, Le Chatelier's principle, relationship between Kp, Kc and Kx for reactions involving ideal gases.

UNIT-3: Ionic Equilibria **(10 Hours)**

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, Ostwald's dilution law, ionization constant and ionic product of water, ionization of weak acids and bases, Degree of ionization, pH scale, common ion effect, Buffer solutions, Henderson-Hasselbach equation. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle

Practical Component: **Credits:02**

(Laboratory periods: 15 classes of 4 hours each)

Chemical Energetics:

1. Determination of heat capacity ofcalorimeter.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodiumhydroxide.
3. Determination of the enthalpy of ionization of acetic acid.
4. Determination of enthalpy of neutralization of acetic acid and ammonium hydroxide using Hess's law.
5. Determination of integral enthalpy of solution (both endothermic and exothermic) of salts.
6. Determination of enthalpy of hydration of Copper sulphate.

Ionic equilibria:

7. Preparation of buffer solutions: (i) Sodium acetate-acetic acid or (ii) Ammonium chloride-ammonium acetate. Measurement of the pH of buffer solutions and comparison of the values with theoretical values.
8. Study the effect of addition of HCl/NaOH on pH of the buffer solutions (acetic acid, and sodium acetate).
9. pH metric titration of strong acid with strong base,
10. pH metric titration of weak acid with strong base

References:

Theory:

1. Castellan, G. W. (2004),**Physical Chemistry**,Narosa.
2. Kapoor, K. L. (2015),**A Textbook of Physical Chemistry**,Vol 1, 6th Edition, McGraw Hill Education.
3. Kapoor, K. L. (2015), **A Textbook of Physical Chemistry**, Vol 2, 6thEdition, McGraw Hill Education.
4. Puri, B. R., Sharma, L. R. and Pathania M. S. (2020), **Principles of Physical Chemistry**, Vishal PublishingCo.

Practical:

1. Khosla,B. D.;Garg,V. C.; Gulati,A.(2015), **SeniorPracticalPhysicalChemistry**,R.Chand&Co.
2. Kapoor, K. L. (2019), **A Textbook of Physical Chemistry**, Vol 7, 1st Edition, McGraw Hill Education.
3. Batra, S. K., Kapoor, V and Gulati, S. (2017) 1st Edition, **Experiments in Physical Chemistry,** Book Age series.

Additional Resources:

1. Mahan, B. H.(2013), **University Chemistry**,Narosa.
2. Barrow, G. M. (2006), **Physical Chemistry**, 5thEdition, McGrawHill.

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

DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -1:

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-1: Chemistry of Major and Minor Biogenic Elements	**04**	**02**	**-**	**02**	**Class XII with Science**	

Learning Objectives

The Learning Objectives of this course are as follows:

- To review periodic properties of main group elements and their role in the biological systems.
- To discuss the patterns and trends exhibited by main group elements and their compounds with emphasis on synthesis, structure, bonding and their diverse applications in the environment, industry and in the biological system.
- To get an insight into how these compounds such as oxides of N and S affect our day-to-day life.
- To learn about inorganic polymeric compounds borazine, silicates, silicones, phosphonitrilic compounds and their applications.
- To develop the interest of students in the frontier areas of inorganic and material chemistry.

Learning outcomes

By studying this course, students will be able to:

- Explain the periodicity in atomic and ionic radii, electronegativity, ionization enthalpy, electron gain enthalpy of elements of the periodic table.
- Explain oxidation states with reference to the existence of elements in unusual and rare oxidation states in alkalides, carbides and nitrides.
- Explain vital role of sodium, potassium, calcium and magnesium ions etc. in biological systems and the role of oxides of N and S in our environment.
- Predict distribution of major and minor biogenic elements in human beings

SYLLABUS OF CHEM-DSE 1

UNIT-1: Periodic Properties **(6 Hours)**

Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, the concept of exchange energy, inert pair effect.
General group trends of main group elements with special reference to size (atomic and ionic), Ionization Enthalpy, Electron Gain Enthalpy, Electronegativity, oxidation states (including rare oxidation states of alkali metals, carbides and nitrides), melting and boiling points, flame colour, metallic character and complex formation tendency (crown ethers and cryptates), Alkali metal solutions in liquid ammonia
Distribution of major and minor biogenic elements in human beings

UNIT 2: Structure, Bonding and Properties **(16 Hours)**

Structure, bonding and properties: Acidic/Basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, thermal stability of the following:
Hydrides: hydrides of Group 13 (only diborane), Group 14, Group 15 (EH_3 where E = N, P, As, Sb, Bi), Group 16 and Group 17.
Oxides: Oxides of nitrogen, phosphorus and sulphur
Oxoacids: oxoacids of phosphorus, sulphur and chlorine
Halides of phosphorus

Relevance of above compounds in industrial/environmental/biological systems wherever applicable

UNIT 3: Preparation, Properties, Structure and Uses **(8 Hours)**

Preparation, properties, structure and uses of the following compounds: Borazine, Silicates, silicones, Phosphonitrilic halides $\{(PNCl_2)_n$ where n = 3 and 4$\}$

Practical component Credit:02

(Laboratory periods: 15 classes of 4 hours each)

Qualitative semi-micro analysis of mixtures containing 2 anions and 2 cations (preferably 7-8 mixtures). Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested: CO_3^{2-}, NO_2^- , S^{2-}, SO_3^{2-}, SO_4^{2-} , $S_2O_3^{2-}$, CH_3COO^-, F, Cl^- , Br^- , I^- ,
NO_3^- , BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+} , Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}.
The mixtures may contain combination of anions/one interfering anion.
Spot tests should be preferred wherever applicable.

References:

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. Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994), **Concepts and Models of Inorganic Chemistry,** John Wiley & Sons.
4. 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.
5. Housecraft, E. H.; Sharpe, A.G. (2018), **Inorganic Chemistry**, 5th Edition, Pearson.

Practicals:

1. Vogel, A.I. (1972), **Qualitative Inorganic Analysis**, Longman.
2. Svehla, G. (1996), **Vogel's Qualitative Inorganic Analysis**, Prentice Hall

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

DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE -2:

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Chem-DSE-2: Polynuclear Hydrocarbons, Pharmaceutical Compounds, UV- Visible & IR Spectroscopy	**04**	**02**	**-**	**02**	**Class XII with Science**	

Learning Objectives

The Learning Objectives of this course are as follows:

- To introduce the chemistry and applications of polynuclear hydrocarbons and heterocyclic compounds.
- Introduction to spectroscopy, an important analytical tool which allows identification of organic compounds by correlating their spectra to structure.

Learning outcomes

By studying this course, students will be able to:

- Understand the fundamentals of polynuclear hydrocarbons and heterocyclic compounds through the study of methods of preparation, properties and chemical reactions with underlying mechanism.
- Gain insight into the basic fundamental principles of IR and UV-Vis spectroscopic techniques.
- Use basic theoretical principles underlying UV-visible and IR spectroscopy as a tool for functional group identification in organic molecules.

SYLLABUS OF CHEM-DSE-2

UNIT-1: Polynuclear Hydrocarbons **(6 Hours)**

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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