**Kuvempu University**
**Department of Chemistry**
**B.Sc. Chemistry V & VI Semesters Syllabus – 2023-2024 (NEP)**
**B.Sc. Course Pattern and Scheme of Examination under NEP approved by UG-BOS in Chemistry held on 08-09-2023**

# **Course Pattern:** B.Sc. Chemistry V & VI Semesters Syllabus

| Semester | Theory code | Hrs/Week | Credits | Practicals code | Hrs/Week | Credits | Total Credits per Semester |
|---|---|---|---|---|---|---|---|
| V | DSC-9<br>DSC-11 | 4<br>4 | 4<br>4 | DSC-10<br>DSC-12 | 4<br>4 | 2<br>2 | **12** |
| | Major- 2 | | | | | | **12** |
| | Cyber Security or Employability Skills | 3 | 3 | - | - | - | **3** |
| | | | | | | **Total** | **27** |
| VI | DSC-13<br>DSC-15 | 4<br>4 | 4<br>4 | DSC-14<br>DSC-16 | 4<br>4 | 2<br>2 | **12** |
| | Major- 2 | | | | | | **12** |
| | Internship | 4 | 2 | - | - | - | **2** |
| | | | | | | **Total** | **26** |
| **Total Credits : V & VI SEMESTERS (27 + 26 = 53)** | | | | | | | |

## Theory and Practicals (B.Sc. in Chemistry V Semester)

DSC - 09 : Selected Topics in Inorganic Chemistry- III
DSC - 10 : Inorganic Chemistry Practicals
DSC - 11 : Selected Topics in Organic Chemistry- III
DSC - 12 : Organic Chemistry Practicals

## Theory and Practicals (B.Sc. in Chemistry VI Semester)

DSC - 13 : Selected Topics in Physical Chemistry- III
DSC - 14 : Physical Chemistry Practicals
DSC - 15 : Spectroscopy
DSC - 16 : Analytical and Industrial Chemistry Practicals

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**Kuvempu University**
**Department of Chemistry**
**B.Sc. Chemistry V & VI Semesters Syllabus - 2023-2024 (NEP)**
**B.Sc. Course Pattern and Scheme of Examination under NEP approved by UG-BOS in Chemistry held on 08-09-2023**

# **Examination Pattern:** B.Sc. Chemistry V & VI Semesters

| Semester | Theory code | Marks | | | Duration of Semester End Examination (hrs) |
|---|---|---|---|---|---|
| | | Semester End Examination | Internal Assessment | Total Marks | |
| V | DSC-9 | 60 | 40 | 100 | 2 |
| | DSC-11 | 60 | 40 | 100 | 2 |
| | **Practical code** | | | | |
| | DSC-10 | 25 | 25 | 50 | 3 |
| | DSC-12 | 25 | 25 | 50 | 3 |
| | Major-2 | - | - | - | - |
| | Cyber Security or Employability Skills | - | - | - | - |
| **Semester** | **Theory code** | **Marks** | | | **Duration of Semester End Examination (hrs)** |
| | | **Semester End Examination** | **Internal Assessment** | **Total Marks** | |
| VI | DSC-13 | 60 | 40 | 100 | 2 |
| | DSC-15 | 60 | 40 | 100 | 2 |
| | **Practical code** | | | | |
| | DSC-14 | 25 | 25 | 50 | 3 |
| | DSC-16 | 25 | 25 | 50 | 3 |
| | Major-2 | - | - | - | - |
| | Internship | - | - | - | - |

## Theory and Practicals (B.Sc. in Chemistry V Semester)

DSC - 09 : Selected Topics in Inorganic Chemistry- III
DSC - 10 : Inorganic Chemistry Practicals
DSC - 11 : Selected Topics in Organic Chemistry- III
DSC - 12 : Organic Chemistry Practicals

## Theory and Practicals (B.Sc. in Chemistry VI Semester)

DSC - 13 : Selected Topics in Physical Chemistry- III
DSC - 14 : Physical Chemistry Practicals
DSC - 15 : Spectroscopy
DSC - 16 : Analytical and Industrial Chemistry Practicals

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**Kuvempu University**
**Department of Chemistry**
**B.Sc. Chemistry V & VI Semester Syllabus – 2023-2024 (NEP)**
**B.Sc. Course Pattern and Scheme of Examination under NEP approved by UG-BOS in Chemistry held on 08-09-2023**

# DISCIPLINE CORE : SEMESTER - V

## DSC-9: Selected Topics in Inorganic Chemistry-III — Theory-60 hours

**UNIT-I: 15 hours**

Chemical Bonding- VSEPR model, shapes of molecules; $ICl_4^-$, $TeF_5^-$, $TeCl_6^{2-}$, $XeF_6$, $SbCl_6^{3-}$, $ReF_7$, $XeF_8^{2-}$, $TaF_8^{3-}$; Bent rules and energetics of hybridization; electronegativity and partial ionic character; Bonds- Multicenter, Synergic and Agostic bonding. Lattice energy: Born-Lande equation, Kapustinskii equation; polarizability and partial covalent character, radius-ratio rules, structures of simple solids, Zintl-isoelectronic relationship in solids. Molecular orbital theory: LCAO and MO diagrams of heteronuclear diatomic (CO, NO. HF, ICl) and triatomic molecules ($CO_2$ and $NO_2^-$).

**UNIT-II: 15 hours**

Chemistry of main group elements-Structure and bondinginboranes, carboranes, metallocarboranes, Wadesrules, borazines, phosphazenes, S,N-compounds. Silicates-Classification, structures, isomorphous replacement, pyroxenes, layered and vitreous silicates, zeolites and molecular sieves.

HSAB concept: Basis of HSAB concept, acid-base strength, hardness and softness, symbiosis, applications of HSAB concept; Acid- base concept in non-aqueous media, reactions in $BrF_3$, $N_2O_4$, anhydrous $H_2SO_4$, $CH_3COOH$. Isopoly and heteropoly acids of W, Mo and V, preparations, properties, structure and applications.

Nanomaterials and Polymers:- Nanomaterials; General characteristics, a brief and elementary account of synthetic methods; bottom-up method, top-down method, examples (detailed mechanism is not required), general applications of nanomaterials. Polymers; Definition, classification, degree of polymerization, expressions for number average and weight average molecular weights. Determination of molar mass of polymers by viscosity method (Ostwald's viscometric method).

**UNIT-III: 15 hours**

M-M bond and metal atom clusters, halide clusters, bonding in $[ReCl_8]^{2-}$. Metal carbonyl clusters-LNCC's and HNCC's. Electron counting in carbonyl clusters, Wades-Mingos and Lauher rules.

Nuclear Chemistry-The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy. Nuclear Models: Shell model-salient features, forms of the nuclear potential, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model. Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of $\alpha$, $\beta^-$, $\beta^+$ and $\gamma$-decay, internal conversion, Auger effect.

**UNIT-IV: 15 Hours**

**Co-ordination Chemistry:** Double salts, complex salts, definition of terms-complex ion, ligand, co-ordination number, coordination sphere. Types of ligands with example-monodentate, bidentate, polydentate, Ambidentate and macro cyclic ligands (crown ethers, porphyrins). Methods of detection of complex formation- conductivity, pH, colour, EAN rule for stabilizing of complexes. Nomenclature of complex compounds. Isomerism in complex compounds: a) Structural isomerism-Ionization isomerism, hydrate isomerism, linkage isomerism and coordinate isomerism, b) Optical and geometrical isomerism in complex compounds with coordination number 4 and 6.

Applications of complex formation in (a) Metallurgy (in the extraction of nickel and gold) (b) Qualitative and quantitative analysis.

**Valance Bond Theory (VBT):** Valence bond theory as applied to complexes- inner and outer orbital complexes. The structure and geometry of the following complexes to be discussed: $[Fe(CN)_6]^{2-}$, $[Fe(H_2O)_6]^{2+}$, $[MnCl_4]^{2-}$, $[Ni(CO)_4]$, $[Cu(NH_3))_4]^{2+}$.
Modification of VBT: Electroneutrality principle of $[Be(H_2O)]^{2+}$ and back bonding effect with respect to $[Ni(CO)_4]$.
**Crystal Field Theory (CFT):** Splitting of d-orbitals in octahedral and tetrahedral fields, effect of weak and strong field ligands, spectrochemical series of ligands, crystal field stabilization energy and calculation of CFSE for different systems.

**References:**


1. Advanced Inorganic Chemistry, 6th edition; F.A. Cotton and G. Wilkinson.
2. Inorganic Chemistry IV edition; J.E. Huheey, E.A. Keiter and R. L. Keiter, Addison; Wesley (1993).
3. Inorganic Chemistry, II edition, D.F. Shriver, P.W. Atkins and C.H. Langford, ELBS; Oxford University Press, 1994.
4. Chemistry of elements; N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann (1997).
5. Concise Inorganic Chemistry, 5th edition; J.D. Lee (1996).
6. Essentials of nuclear chemistry, 4th edition; H.J. Arniker, NAIL publishers (1995).
7. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller.
8. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald. A. Tarr (2007).
9. Principles of Inorganic Chemistry (UGC Syllabus), B.R. Puri, L.R. Sharma, K.C. Kalia, Milestone Publishers, New Delhi, India, 2008.
10. Advanced Inorganic Chemistry by Gurudeep Raj and Chatwal Anand.
11. Modern Inorganic Chemistry by R.D. Madan.
12. Advanced Inorganic Chemistry by Sathyaprakash.


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## DSC-10: Inorganic Chemistry Practicals 60 hours

**PART-A: Gravimetric and Volumetric Analysis**

1. Gravimetric determination of Fe in iron ore as $Fe_2O_3$.
2. Gravimetric estimation of calcium as calcium oxide.
3. Gravimetric estimation of aluminum as aluminum oxide.
4. Gravimetric estimation of magnesium as magnesium-oxinate.
5. Gravimetric determination of Ni using DMG in Cu and Ni solution.
6. Gravimetric determination of Fe using $NH_4OH$ in Fe and Cr solution.
7. Gravimetric estimation of Cu using $NH_4SCN$ in Cu and Zn solution.
8. Volumetric estimation of Ca and Mg in dolomite solution.
9. Volumetric estimation of Fe in Cu and Fe solution.

**PART-B: Preparation of co-ordination complexes**

1. Preparation of hexamminenickel(II) chloride.
2. Preparation of Cis- and trans-potassium dioxalatodiaquachromium(III)complex [Estimation of oxalate and chromium].
3. Preparation of tris(oxalato)ferrate(III).
4. Preparation of hexamminecobalt(III)chloride(demonstration).
5. Preparation of mercury tetrathiocyantocobaltate(II) (demonstration).
6. Preparation of trans-potassium diaquadioxalatochromate (III).
7. Preparation of tris(thiourea) copper (I) sulphate monohydrate
8. Preparationofpentamminechlorocobalt(III)chloride.

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***Note:*** *The list of experiments is suggestive. However, faculties / academic bodies may add more experiments / references or incorporate suitable revisions based on infrastructure facilities available at the Institution.*

## DSC-11: Selected Topics in Organic Chemistry-III Theory-60 hours

**UNIT-I: 15 hours**

**Alcohols: (8 hours)**

**Monohydric alcohol:**- Classification, nomenclature, preparation from alky halides, aldehydes, ketones. Distinguish test between $1^o$, $2^o$, $3^o$ alcohols by Victor-Meyer method, Lucas method. Test for hydroxyl alcohol- formation of alkoxide, esterification with mechanism, oxidation.

**Dihydric alcohol:**- Nomenclature, preparation of glycol from alkene. Oxidative cleavage using lead tetra acetate, periodic acid.Uses of ethylene glycol.

**Trihydric alcohol:**- Nomenclature, manufacture of glycol from Spent lye. Synthesis from propene. Reactions of glycol with oxalic acid at different temperatures, reaction with $PCl_5$, with fatty acids. Uses of glycerol, preparation of nitroglycerine, composition and uses of Cordite and dynamite.

**Phenols: (7 hours)**

Classification, nomenclature, Methods of preparation from Cumene, Dow process, from diazonium salts.Acidity of phenols- resonance, stabilization of phenoxide ion, compare the acidity of alcohol and phenol. Effect of substituent's on acidity of phenols, electron withdrawing groups ($-NO_2$, -Cl, -CN, -CHO, -COOH), electron donating groups ($-CH_3$, $-OCH_3$, $-NH_2$).

Reactions of phenols. Fries, Claisen, Reimerr-Tiemann, Leader-Manase reactions with mechanism.Synthesis of phenolphthalein, salicylaldehyde, vanillin, o-benzoquinone.

**Unit-II: 15 hours**

**Aldehydes and Ketones: (5 hours)**

Nomenclature. Structure and reactivity of carbonyl groups in aldehydes, ketones.

Reactions of aldehydes and ketones with hydroxyl amine, hydrogen cyanide, 2,4-DNP. Reaction Mechanism of Aldol, Perkin's, Benzoin, Cannizaro, Knoevenagel reaction. Clemmenson reduction, Wolff-Kishner reduction.

**Rearrangements: (5 hours)**

Wolff, Hofmann, Curtius, Lossen and Schmidt rearrangements. Benzil-benzilic acid rearrangement. Stevens, Wittig and Favorskii rearrangements, Baeyer-Villiger oxidation. Neberre arrangement. Benzidine rearrangement.

**Amino acids and proteins: (5 hours)**

Definitions and classification of amino acids, synthesis of amino acids by Gabriel phthalimide, malonic ester and Strecker's method of synthesis.

Properties and reactions- Zwitter ion and isoelectric points. Ninhydrin and Biuret tests.

Peptides: peptide bond, carbobenzoxy method of synthesis of peptides.

Proteins: Classification based on composition and structure: primary and secondary structures of proteins. Denaturation of proteins.

**UNIT-III: 15 hours**

**Stereochemistry: (6 hours)**

Walden inversion, asymmetric synthesis.Geometrical isomerism: Geometric isomerism in maleic acid and fumaric acid. Determination of their configurations. Geometrical isomerism of oximes, Determination of configuration of oximes. Beckmann rearrangement.

Conformational analysis: Conformational analysis of cycloalkanes : cyclobutane, cyclopentane, cyclohexanes (monosubstituted e.g., methyl, iso-propyl, tert-butyl and di-substituted cyclohexanes e.g., dialkyl, dihalo, diols), and cycloheptane.

**Carbohydrates: (6 hours)**

Introduction, Kiliani-Fischer synthesis, Determination of configuration of the monosaccharides, conformational analysis of monosaccharides. Synthesis of amino sugars (β-D-Glucosamine, galactosamine, N-acetylmuramic acid (NAMA), N-acetylneuraminic acid NANA). C-and N-glycosides. Synthesis of aldonic, uronic, aldaric acids and alditols. Structure elucidation of sucrose and maltose. Structures of lactose, gentiobiose, and meliobiose. Photosynthesis of carbohydrates.

**Retrosynthesis: (3 hours)**
Retrosynthesis of benzocaine, 4-methoxy acetophenone, saccharin. Disconnection approach. General terms: synthon, synthetic equivalents and target molecule. General guidelines for disconnection.

**Unit-IV:** **15 hours**

**Heterocycliccompounds:**
Nomenclature of heterocyclic compounds. Preparation and reactions of pyrrole, furan, thiophene, indole, pyridine, quinoline, isoquinoline. Aromaticity of pyrrole, furan, thiophene. Basicity of pyrrole and pyridine.
Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyrimidine, purine. Preparation and reactions of coumarins, acridines, cinnolenes and quinoxalines.

**References:**

1. Advanced Organic Chemistry- Reactions, Mechanism and Structure, Jerry March, JohnWiley (2008).
2. Advanced Organic Chemistry, FA Carey and RJ Sundberg Plenum,(1990).
3. A Guide Book to Mechanismin Organic Chemistry, Peter Sykes, Longman, (2000).
4. Structure and mechanism of Organic Chemistry, CK Ingold, Cornell University Press (1999).
5. Organic Chemistry, RT Morrison and RN Boyd, Prentice-Hall, (1998).
6. Modern Organic Reactions, HO House, Benjamin, (1972).
7. Principles of Organic Synthesis, ROC Norman and JM Coxon, Blackie Academic and Professional, (1996).
8. Stereochemistry of Organic Compounds, D Nasipuri, New-Age International, (1999).
9. Stereochemistry of Carbon Compounds, ELEliel, SH Wilenand LN Mander, JohnWiley, (1994).
10. Stereochemistry,Potapov, MIR, Moscow,1984.
11. Organic Chemistry, Volumes I and II, IL Finar, Longman,(1999).
12. Organic Chemistry, Bahl and ArunBahl, S. Chand and Sons, New Delhi, 2005.
13. Organic Chemistry, R. T. Morrison and R. N. Boyd, VI Edition, Printice-Hall of India Limited, New Delhi, 1992.
14. Organic Chemistry, B. Y. Paula, III Edition, Pearson Education, Inc.(Singapore), New Delhi, reprint, 2002.
15. Textbook of Organic Chemistry, P S Kalsi, Mac Millan, 2000.


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## DSC-12 : Organic Chemistry Practicals 60 hours

**PART-A : Preparation (one stage)**

1. Cannizarroreaction: Benzaldehyde.
2. Friesrearrangement: Phenylacetate.
3. Friedel-Craftsreaction: Benzeneand Acetylchloride.
4. Sandmeyerreaction: 4-Chlorotoluene from 4-toluidine.
5. Pechmannreaction: Resorcinol and ethylacetoacetate.
6. Oxidation of Cyclohexanol.
7. Preparation of S-Benzylisothiuronium chloride.
8. Synthesis of p-iodonitrobenzene
9. Synthesis of N-Phenyl-2,4-dinitroaniline.
10. Synthesis of 2,4,6-tribromoaniline.
11. Synthesis of 2,4-dichlorophenoxy acetic acid.

**PART-B : Organic Estimations (Quantitative analysis):**

1. Titrimetric estimation of aminoacids.
2. Determination of saponification value of oil.
3. Estimation of glucose by Fehling's method.
4. Estimation of keto group.
5. Estimation of phenol.
6. Estimation of aniline.
7. Iodine value of oil by chloramine-T method.

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***Note:*** *The list of experiments is suggestive. However, faculties / academic bodies may add more experiments / references or incorporate suitable revisions based on infrastructure facilities available at the Institution.*

## Course outcomes (V-Semester):

After the completion of this course, the student would be able to,

1. Predict bonding in molecules/compounds/ions, multi centered bonds.
2. Understand the properties of ionic compounds, like, Lattice energy and also the MO diagrams of different types of molecules.
3. Learn the important features of some of the compounds of main group elements.
4. Know the HSAB Concepts of acid, bases and they will learn the basics of nanomaterials and polymers.
5. Develop a thorough knowledge on the fundamentals bonding in metal atom clusters, various concepts/models in nuclear chemistry and radioactivity.
6. Explain the broad and balanced ideas on the important concepts in Co-ordination Chemistry, application of theories to the complex compounds.
7. Predict the key concepts about the Classification, nomenclature, preparation, reactions of alcohols and phenols.
8. Acquire the thorough knowledge on Nomenclature, Structure and reactivity of carbonyl groups in aldehydes, ketones and certain rearrangement reactions.
9. Give the classification and properties of amino acids, structure properties and reactions of peptides and Proteins.
10. Understand the concept of stereochemistry and its importance will be taught with respect to the structural analysis.
11. Explain the fundamentals of structure, reactions and synthesis of Carbohydrates.
12. Learn general terms and guidelines for disconnection approach in retrosynthesis.
13. Develop an idea about the nomenclature, Structure, reactivity and synthesis of various heterocyclic compounds.
14. Acquire the ability to plan and carryout experiments on Gravimetric and Volumetric Analysis and Preparation of various co-ordination complexes under different conditions and using specific reagents independently and assess the significance of outcomes.
15. To plan and carryout the experiments on Practical knowledge on one step preparation of important organic compounds and Quantitative analysis/estimation of organic compounds and to cater to the demands of chemical Industries of well-trained graduates.

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# DISCIPLINE CORE : SEMESTER - VI

## DSC-13: Selected Topics in Physical Chemistry-III Theory-60 hours

**Unit-I: 15 hours**

**Electrochemistry-II: (6 hours)**

Definition of EMF of a cell, standard electrode potential, IUPAC sign convention; Types of reversible electrodes with examples: gas-metal ion, metal-ion, metal insoluble salt-anion electrode, Redox electrode with examples – Quinhydrone electrode (To be mentioned).

Reference electrodes – Construction and working of SHE and calomel electrode. Concentration cell – Derivation of EMF using Nernst equation for electrolytic concentration cell without transference. Liquid junction potentials, elimination of liquid junction potential. Potentiometric titration involving only redox systems ($K_2Cr_2O_7$vs. FAS).

**Quantum Mechanics: (9 hours)**

Physical interpretation of the wave function. Operators: Laplacian, Hamiltonian, Linear and Hermitian operators. Angular Momentum operators and their properties. Commutation of operators. Postulates of quantum mechanics, Schrödinger wave equation based on the postulates of quantum mechanics and its importance. Concepts of solutions of Schrödinger wave equation for a Particle in a one dimensional box, particle in a three-dimensional box. Quantum mechanical degeneracy, tunneling (no derivation). Application of Schrödinger equation to harmonic oscillator, rigid rotator. Eigen functions and eigen values of angular momentum. Ladder operator method for angular momentum. Schrödinger equation to hydrogen atom in spherical polar co-ordinates. Total wave functions of hydrogen atom. Quantum numbers and their characteristics. List of wave functions for few initial states of hydrogen like atoms.

**UNIT-II: 15 hours**

**Chemical Dynamics-I**

Macroscopic and microscopic kinetics, Review of theories of reaction rate-Collision theory and Transition state theory, Comparison of collision theory with transition state theory, Arrhenious equation-characteristics, Significance of energy of activation, Temperature coefficient and its evaluation. Thermodynamical formulation of reaction rates (Wyne-jones and Eyring treatment), Reaction between ions in solutions – Influence of ionic strength on reaction rates (primary and secondary salt effects).

**Concept of Steady state kinetics**, Chain reactions - chain length and chain inhibition, comparison ofphotochemical and thermal reactions, Mechanisms of thermal and photochemical reactions between hydrogen-bromine and hydrogen-chlorine. Comparative study of thermal and photochemical hydrogen-halogen reactions. Pyrolysis of acetaldehyde, Decomposition of ethane.

Kinetics of fast reactions- Introduction, Study of reactions by relaxation method (Temperature andpressure jump), flow method (Plug flow method and Stopped flow method), Flash photolysis and Shock tube method.

**UNIT-III: 15 hours**

**Chemical Dynamics-II**

Kinetics of homogeneous catalysis-kinetics of auto catalytic reactions, kinetics of acid-base catalysed reactions. Comparison of enzyme catalysed and chemical catalysed reactions, Mechanism (Lock and Key theory), Kinetics of enzyme catalyzed reactions - Henri-Michaelis- Menten mechanism, Significance of Michaelis-Menten constant, Lineweaver-Burk plot. Effects of enzyme concentration, pH, Temperature, Activators and Inhibitors on enzyme activity.

Theories of unimoleuclar reactions: Perrin theory and Hinshelwood theory.

Surface chemistry- Adsorption: Effect of temperature on adsorption, Mechanism of adsorption, Derivation of BET equation, Estimation of surface area using BET equation, Gibbs adsorption isotherm and its significance, Surface tension and surface energy, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Surface film on liquids (electro-kinetic phenomena), Catalytic activity of surfaces.

**UNIT-IV:** **15 hours**

**Thermodynamics:** Nernst heat theorem; statement and concept of residual entropy, evaluation of absolute entropy, Third law of thermodynamics. Entropy of vapourisation and Trauton's rule, limitations of Van't Hoff's equation. Fugacity - its variation and determination, activity and activity coefficient. Partial molar quantities; Concept of chemical potential, variation of chemical potential with temperature and pressure, derivation of Gibbs-Duhem equation, Duhem-Margules equation and its application.

**Phase Rule:** Derivation of phase rule from the concept of chemical potential. Application of Phase Rule to three components system: Principle of triangular diagram: Plots for a mixture of three liquids consisting of one, two and three pairs of partially miscible liquids.

**Statistical Thermodynamics:** Energy states: macro and microstates, Limitation of classical thermodynamics, Distinguish between classical mechanics and statistical mechanics. Sterling approximation, derivation of Maxwell–Boltzmann statistics, statistical interpretation of entropy, application of statistics to gases-monoatomic ideal gas (No derivations). Partition functions and thermodynamic parameters, expressions for translational, rotational, vibrational and electronic partition functions, enthalpy, energy, Gibbs free energy.

**Partition functions:** Definition and significance, molar and molecular partition functions, Derivation of expression of partition function for rotational, vibrational, electronic, and translational motion. Sackur Tetrode Equation, Relation between equilibrium constant and partition function.

**References:**


1. Physical Chemistry, P.W. Atkins, Juliode Paula, ELBS, 7th edition, (2002).
2. Physical Chemistry: A Molecular Approach, McQuarie and Simon, Viva, New Delhi, (2001).
3. Introduction to Quantum Chemistry, A.K. Chandra,Tata McGraw Hill, (1988).
4. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
5. Quantum Chemistry, R.K. Prasad, New Age International, 2nd edition, (2000).
6. Quantum Chemistry through problems and solutions, R.K. Prasad, New Age International (1997).
7. Chemical Kinetics- K.J. Laidler, McGraw Hill. Inc. New York (1988).
8. Principles of Chemical Kinetics – House J.E. Wm C Brown Publisher, Boston, (1997).
9. Kinetics and Mechanism - A.A. Frost and R.G. Pearson, John-Wiley, New York, (1961).
10. Chemical Kinetic Methods - C. Kalidas, New Age International Publisher, New Delhi (1995)
11. S.H. Maran and C.F. Pruton, 4th Edn., Oxford, and IBH publishing Co. Pvt. Ltd. New Delhi (1965).
12. Principles of Physical Chemistry: Puri, Sharma and Pathania, Vishal Publishing House.
13. Essential of Physical Chemistry; Arun Bahl, B.S. Bahi and G.D. Tuli, S. Chand and Co.
14. Physical chemistry; R. L. Madan, G. D. Tuli, S. Chand and Co.
15. Elements of Physical Chemistry - Glasstone and Lewis - Macmillan.
16. Text book of Physical Chemistry - S. Glasstone- Macmillan (India) Ltd.
17. Numerical Problems on Physical Chemistry- Gashal, Books and Allied (P) Ltd.,
18. Physical Chemistry, P. C. Rakshit, V Edition (1988), Fourth Reprint (1997), Sarat Book House, Calcutta.
19. W. Kauzmann, Kinetic Theory of Gases (Thermal Properties of Matter, Vol I), Benjamin, Reading, MA, 1966.


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## DSC-14: Physical Chemistry Practicals 60 hours

**PART-A:**

1. Conductometric titration of weak acid versus weak base.
2. Conductometric titration of solution of strong acid (HCl) and salt ($CuSO_4$) versus Strong Base.
3. Potentiometric titration of FAS versus $K_2Cr_2O_7$.
4. Potentiometric titration of FAS versus $KMnO_4$.
5. Potentiometric method of determination of dissociation constant of $H_3PO_4$.
6. Potentiometric titration of weak acid against a strong base using quinhydrone electrode and calculation of $pK_a$ and $K_a$ of the weak acid.
7. Determination of the acidic and basic dissociation constant and isoelectric point of an amino acid by *p*H-metry.

**PART-B:**

1. Determination of rate constant of hydrolysis of ester in presence of two different concentrations of catalyst (HCl).
2. Determination of rate constant of hydrolysis of ester catalyzed by HCl at different temperatures.
3. Determination of rate constant of decomposition of Hydrogen peroxide catalyzed by $FeCl_3$.
4. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and calculation of dissociation constant of the base by *p*H-metry.
5. Analysis of a binary mixture of two miscible liquids and to determine the composition of the given unknown mixture by Abbe's refractometry.
6. Determination of *p*H of acetic acid with sodium acetate buffer by *p*H-metry method.
7. Colorimetric estimation of $Fe^{2+}$ ions using 1,10-phenothralene.

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***Note:*** *The list of experiments is suggestive. However, faculties / academic bodies may add more experiments / references or incorporate suitable revisions based on infrastructure facilities available at the Institution.*

## DSC-15 : SPECTROSCOPY — Theory - 60 hours

**Unit-I:** **15 hours**

**Symmetry and Group Theory in Chemistry: (7 hours)**

Definition of groups, sub-groups, cyclic groups, conjugate relationships, classes, simple theorems in group theory. Symmetry elements and symmetry operations, point groups, Schöenflies notations, representations of groups by matrices, reducible and irreducible representations, characters of representations, Great Orthogonality Theorem (without proof) and its applications, group multiplication tables for $C_{2v}$ (Example : water) $C_{3v}$ (Example : ammonia), character tables for $C_n$ (consider $C_2$ and $H_2O_2$ as an example for $C_2$ point group), $C_{nv}$ (consider $C_{2v}$ and water as an example for $C_{2v}$ point group), $D_{nh}$ (consider $D_{3h}$ and $BF_3$ as an example for $D_{3h}$ point group) point groups to be worked out.

**Molecular spectroscopy : (8 hours)**

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

**Raman spectroscopy:** Theory, Qualitative treatment of Rotational Raman effect; Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion. Relation with IR spectroscopy, Instrumentation.

**Vibrational spectroscopy:** Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies. Fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, PQR branches.

**Unit-II:** **15 hours**

**Organic Spectroscopy:**

General principles, Introduction to absorption and emission spectroscopy.

**UV Spectroscopy:** Types of electronic transitions, $\lambda_{max}$,Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of $\lambda_{max}$ for the following systems: α,β unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between cis and trans isomers.

**IR Spectroscopy:** Fundamental and non-fundamental molecular vibrations; Range, finger print region, and its significance; frequency and energy of IR radiations, interaction of IR radiation with organic molecules, molecular vibrations- stretching and bending vibrations, Hook's law, Stretching frequency of functional groups in benzaldehyde, acetophenone, ethyl acetate, aniline and methyl amine. Infrared spectra of simple molecules, C=C stretching and –C=H bending vibrations in vinyl ethers. Calculation of vibrational frequencies using Hooke's law derived for the motion of a spring. Sample handling in IR spectra of both gases and liquids.

**Unit-III:** **15 hours**

**Nuclear Magnetic Resonance spectroscopy:**

Nuclear magnetic resonance (NMR) spectroscopy: Absorption of electromagnetic radiation, proton NMR ($^1$H NMR) , Magnetic properties of nuclei, population of energy levels, the Larmor precession, relaxation processes, chemical shift, the relationship between number of signals and their ratio, shielding mechanism, spin-spin interactions, rules governing the interpretation of first order spectra, effect of chemical exchange on spectra. NMR spectra: Downfield and up field position of a signal and integral curve. $^1$H NMR spectrum of organic molecules like ethanol, p-xylene. Factors influencing chemical shift, anisotropic effect.

**Atomic spectroscopy**: Atomic absorption, atomic emission and atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

**Unit-IV:** **15 hours**

**Mass Spectrometry:** Basic principles- Theory of mass spectrometry, instrumentation, mass spectrum, the molecular ion peak, determination of molecular formula, Mc-Lafferty rearrangement. Metastable ion peaks and their importance. Nitrogen rule. General transformation modes. Homolytic cleavage heterolytic cleavage. Retro-Deil's Alder reactions. Important features of mass spectra of hydrocarbons - alkanes, alkenes and cycloalkenes, alcohols, phenols, aldehydes, ketones, carboxylic acids.

**Electron Paramagnetic Resonance (EPR) Spectroscopy**: Basic principles, selection rules, intensity, width, position of spectral line, multiplet structure of EPR spectra, hyperfine interaction, spin-orbit coupling, zero field splitting and Kramer's degeneracy, rules for interpreting spectra, factors affecting the magnitude of values. Instrumentation, applications to the study of free radicals, coordination compounds, biological studies and rate of electron exchange reactions.

**Nuclear Quadrupole Resonance (NQR) Spectroscopy:** Quadrupole nuclei, quadrapole movement, electric field gradient, the NQR experiment, structural information from NQRspectra.

**References:**


1. Chemical Applications of Group Theory, F. A. CoZon, Wiley Eastern (1976).
2. Molecular Symmetry, D. S. Schonl and, Van Nostr and (1965).
3. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH EdiBon (1994).
4. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (Int. Students Edition) (1988).
5. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (Int. Students EdiBon) (1990).
6. Spectroscopy, Vols. 1-3, B. P. Straughan and W. Walker, Chapman Hall (1976).
7. Physical Methods in Chemistry – R.S. Drago, Saundercollege.
8. Structural Methods in Inorganic Chemistry – E.A. Ebsworth, D. W.H. Ranbin and S.Cradock, ELBS.
9. Spectra of Inorganic and Coordination Compounds - K. Nakamoto.
10. Infrared Spectroscopy - C.N.R. Rao.
11. Introduction to Spectroscopy - D.L. Pavia, G.M. Lampman and G.S. Kriz, Thomson Learning, Singapore (2001).
12. Spectroscopic Identification of organic compounds - R.M. Silverstein and F.X. Webster, 6$^{th}$ Edition, John Wiley and Sons, India Ltd. (2006).
13. Interpretation of Mass Spectroscopy – Mc Lafferty.
14. Organic Spectroscopy, William Kemp.


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## DSC-16 : Analytical and Industrial Chemistry Practicals 60 hours

**Part-A: Separation techniques and pharmaceutical analysis**

1. Separation of amino acids by paper chromatography and measuring $R_f$ values.
2. Separation of $Co^{2+}$ and $Ni^{2+}$ by paper chromatography and measuring $R_f$ values.
3. Separation of Ni(II) and Fe(II) by complexation with DMG, extraction of Ni(II)-DMG complex in chloroform and determination of its concentration by colorimetry.
4. Separation of amino acids from organic acids by ion exchange chromatography,
5. Separation of Mg (II) and Fe (II) by ion exchange chromatogrphy.
6. Determination of aspirin present in tablets conductometrically / titrimetrically
7. Determination of amino acids colorimetrically using ninhydrin.
8. Determination of Glucose / Sucrose colorimetrically using Fehling's Solution.
9. Preparation of magnesium bisilicate (Antacid).

**Part-B: Industrial Chemistry**

1. Safety practices in the Chemistry laboratories.
2. Determination of calcium in fertilizer.
3. Determination of water of crystallization and Fe(II) in Mohr's salt by titrating with standard $KMnO_4$.
4. Preparation of phenol formaldehyde Resin.
5. Preparation of urea formaldehyde resin.
6. Nitration of salicylic acid by green method (Using calcium nitrate and acetic acid).
7. Preparation of aspirin from salicylic acid.
8. Analysis of Cement [Moisture, Silica and Calcium (II)].
9. Analysis of food adulterants in Tea Powder, Coffee Powder, turmeric powder, Chili Powder, oil/fat, milk, etc.
10. IR peak analysis for functional groups using recoded IR Spectra.
11. Preparation and characterization of biodiesel from vegetable oil/waste cooking oil.

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***Note:*** *The list of experiments is suggestive. However, faculties / academic bodies may add more experiments / references or incorporate suitable revisions based on infrastructure facilities available at the Institution.*

## Course outcomes (VI-Semester):

After the completion of this course, the student would be able to,

1. Understand the electrochemical aspects types of electrodes, their construction and working, liquid junction potentials and potentiometric titrations.
2. Learn the fundamentals of Quantum Mechanics, application of the Schrödinger equation to various systems.
3. Understand the concepts of macroscopic and microscopic kinetics, thermodynamical formulation of reaction rates, steady state kinetics and fast reactions.
4. Acquire a thorough knowledge on the topics on Kinetics of homogeneous catalysis, theories involved and the various concepts in surface chemistry.
5. Know the basic concepts of entropy and the Third law of thermodynamics, partial molar properties and their applications in problem solving skills.
6. Understand the Phase rule and to distinguish between phase diagrams of various systems consisting of one, two and three pairs of partially miscible liquids.
7. Explain the concepts in statistical thermodynamics, derivation of statistical equations of distribution laws, partition functions and their applications, develop problem solving skills.
8. Develop an idea of various concepts in Symmetry and Group Theory, including definitions, symmetry elements, symmetry operations and group multiplication tables with specific examples (as Symmetry and Group Theory is the basis for many spectroscopic studies).
9. Understand and to explain the fundamentals of Molecular spectroscopy, which involves the Interaction of electromagnetic radiation with molecules explanation about different types of molecular spectra like Rotation spectroscopy,Raman spectroscopy and Vibrational spectroscopy.
10. Explain the general principles, Introduction to absorption and emission spectroscopy, particularly about the fundamentals of UV Spectroscopy and IR Spectroscopy.
11. Utilize the concepts in Nuclear magnetic resonance (NMR) spectroscopy, magnetic nuclei, NMR signals of simple molecules and also the fundamental knowledge ofAtomic spectroscopy.
12. Know the important principles involving, theory of mass spectrometry, instrumentation, mass spectrum, the molecular ion peak, determination of molecular formula, important features of mass spectra of some molecules.
13. Understand the basic principles, selection rules, intensity, width, position of spectral line, multiplet structure of EPR spectra, instrumentation and applications.
14. Learn the fundamentals of NQR, NQR experiment, structural information from NQR spectra.
15. To plan and carryout experiments on Conductometrictitration and potentiometric titrations involving neutralization and redox reactions, Abbes refractometry, pH metry and colorimetry and to understand the basic knowledge on these experiments.
16. Obtain the ability to plan and carryout experiments independently on Separation techniques involving chromatography and to cater to the demands of chemical Industries.

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# Question paper pattern for FIFTH and SIXTH Semesters

Paper Title and Code:

Time: 2 hrs] [Max. Marks: 60

***Instructions to all candidates* :**

1. **The question paper contains Four sections A, B, C and D. Answer all Sections.**
2. **Section A contains multiple choice questions and should be answered in the first two pages of main answer book. The questions of section – A answered in any other part of the book will not be valued.**
3. **Write equations and neat diagrams wherever necessary.**

## SECTION – A

**Each one of the following questions is provided with four answers a, b, c and d. Choose the correct answer among them and write it along with the respective answer in the main answer book.** **10 ×1=10 Marks**

**1.**

**i) ……..**
**a). b). c). d).**

**ii) ……..**
**a). b). c). d).**

**iii) ……..**
**a). b). c). d).**

**iv) ……..**
**a). b). c). d).**

**v) ……..**
**a). b). c). d).**

**vi) ……..**
**a). b). c). d).**

**vii) ……..**
**a). b). c). d).**

**viii) ……..**
**a). b). c). d).**

**ix) ……..**
**a). b). c). d).**

**x) ……..**
**a). b). c). d).**

## SECTION – B

**Answer any FIVE of the following questions :** **5 × 3 =15 Marks**

**2. ……..** **6. ……..**

**3. ……..** **7. ……..**

**4. ……..** **8. ……..**

**5. ……..** **9. ……..**

## SECTION – C

**Answer any THREE of the following questions :** **3 × 5 =15 Marks**

**10. a)……..**
**b)……..**
**11. a)……..**
**b)……..**
**12. a)……..**
**b)……..**
**13. a)……..**
**b)……..**
**14. a)……..**
**b)……..**

## SECTION – D

**I. Answer the following questions :** **2 × 10 = 20 Marks**

**15. a) i) …….** **a) i)……**
**ii) …….** **‹ ›** **ii)…….**
**iii) …….**

**OR**

**b) i) …….** **a) i)……**
**ii) …….** **‹ ›** **ii)…….**
**iii) …….**

**16. a) i) …….** **a) i)……**
**ii) …….** **‹ ›** **ii)…….**
**iii) …….**

**OR**

**b) i) …….** **a) i)……**
**ii) …….** **‹ ›** **ii)…….**
**iii) …….**

**Note :** Questions 15 & 16 may be sub-divided into **a) i), ii), iii), b) i), ii), iii) OR a) i), ii), b) i), ii) carrying 3+3+4, 2+4+4 OR 3+7, 4+6, 5+5 marks** depending on the weightage of the questions.

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## Note:

| Internal Assessment for Theory Papers | |
|---|---|
| **Mode of Assessment** | **Marks** |
| Internal Assessment Test-1 | 10 |
| Internal Assessment Test-2 | 10 |
| Quiz/Assignment/Small Project | 10 |
| Seminar | 10 |
| **Total** | **40** |

| Internal Assessment for Practical Papers | |
|---|---|
| **Mode of Assessment** | **Marks** |
| Internal Assessment Test | 10 |
| Practical Record | 15 |
| **Total** | **25** |

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