B.Sc. (H) Chemistry

THREE-YEAR FULL-TIME PROGRAMME
(Six-Semester Course)

COURSE CONTENTS

(Effective from the Academic Year 2010-2011)

UNIVERSITY OF DELHI

DELHI – 110 007

Course Structure

YEAR-1

PART I: Semester – 1

Paper 1	CHHT 101	Inorganic Chemistry- I
Paper 2	CHHT 102	Organic Chemistry –I
Paper 3	ENAT 101	Technical writing and Communication in English
Paper 4	MACT 101	Mathematics-I

PART I: Semester – 2

Paper 5	CHHT 203	Physical Chemistry – I
Paper 6	CHHT 204	Analytical Methods in Chemical Analysis
Paper 7	LSPT 202	Biology-II
Paper 8	PHCT 201	Physics-I

In addition, there shall be one qualifying paper in self-learning mode called Environmental Studies offered in Semester-2

YEAR-2

PART II: Semester – 3

Paper 9	CHHT 305	Inorganic Chemistry – II
Paper 10	CHHT 306	Organic Chemistry – II
Paper 11	CHHT 307	Physical Chemistry – II
Paper 12	MACT 302	Mathematics-II

PART II: Semester – 4

Paper 13	CHHT 408	Inorganic Chemistry – III
Paper 14	CHHT 409	Organic Chemistry – III
Paper 15	CHHT 410	Physical Chemistry – III
Paper 16	PHCT 402	Physics-II

YEAR-3

PART III: Semester – 5

Paper 17	CHHT 511	Inorganic Chemistry – IV
Paper 18	CHHT 512	Organic Chemistry – IV
Paper 19 a/b	CHHT 513	Physical Chemistry – IV
Paper 20	CHHT 514	Biochemistry and Environmental Chemistry

PART III: Semester – 6

Paper 21	CHHT 615	Inorganic Chemistry – V
Paper 22	CHHT 616	Organic Chemistry – V
Paper 23	CHHT 617	Physical Chemistry – V
Paper 24	CHHT 618	Applications of Computers in Chemistry

Paper 1-CHHT 101: Inorganic Chemistry - I

THEORY **Marks: 100**

Unit I: Atomic Structure:

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's uncertainty principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance. Normal and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Contour boundary and probability diagrams.

Pauli's exclusion principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

Unit II: Periodicity of Elements:

s, p, d, f block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to s & p- block.

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.
(b) Atomic radii (van der Waals)
(c) Ionic and crystal radii.
(d) Covalent radii (octahedral and tetrahedral)
(e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy.
(f) Electron gain enthalpy, trends of electron gain enthalpy.
(g) Electronegativity, Pauling's/ Mulliken's/ Allred Rachow's/ and Mulliken-Jaffe's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.

Recommended Texts:

1. Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
2. Douglas, B.E. and Mc Daniel, D.H., *Concepts & Models of Inorganic Chemistry*, Oxford, 1970
3. Atkins, P.W. & Paula, J. *Physical Chemistry*, Oxford Press, 2006.
4. Day, M.C. and Selbin, J. *Theoretical Inorganic Chemistry*, ACS Publications 1962.

Paper 2-CHHT 102: Organic Chemistry - I

THEORY   **Marks: 100**

Unit-I: Basics of Organic Chemistry

Organic Compounds: Classification, and Nomenclature, Hybridization, Shapes of molecules, Influence of hybridization on bond properties.

Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and their applications; Dipole moment; Organic acids and bases; their relative strength.

Homolytic and Heterolytic fission with suitable examples. Curly arrow rules, formal charges; Electrophiles and Nucleophiles; Nucleophlicity and basicity; Types, shape and their relative stability of Carbocations, Carbanions, Free radicals and Carbenes

Introduction to types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions.

Unit II: Stereochemistry

Fischer Projection, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: cis–trans and, syn-anti isomerism E/Z notations with C.I.P rules.

Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral-centres, Distereoisomers, meso structures, Racemic mixture and resolution. Relative and absolute configuration: D/L and R/S designations.

Unit III: Chemistry of Aliphatic Hydrocarbons

A.   Carbon-Carbon sigma bonds

Chemistry of alkanes: Formation of alkanes, Wurtz Reaction, Wurtz- Fittig Reactions, Free radical substitutions: Halogenation - relative reactivity and selectivity.

B.   Carbon-Carbon pi bonds

Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations.

Reactions of alkenes: Electrophilic additions their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroboration-

oxidation, ozonolysis, reduction (catalytic and chemical), syn and anti hydroxylation (oxidation). 1, 2- and 1, 4- addition reactions in conjugated dienes and, Diels-Alder reaction; Allylic and benzylic bromination and mechanism, e.g. propene, 1-butene, toluene, ethyl benzene.

Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

C.   Cycloalkanes and Conformational Analysis

Types of cycloalkanes and their relative stability, Baeyer strain theory, Conformation analysis of alkanes: Relative stability: Energy diagrams of cyclohexane: Chair, Boat and Twist boat forms; Relative stability with energy diagrams.

Unit IV: Aromatic Hydrocarbons

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples. Electrophilic aromatic substitution: halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the groups.

Recommended Texts:

1. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, 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: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

4. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*; Wiley: London, 1994.

Paper 3-ENAT 101: TECHNICAL WRITING AND COMMUNICATION IN ENGLISH

Marks: 100

Unit 1

Communication: Language and communication, differences between speech and writing, distinct features of speech, distinct features of writing.

Unit 2

Writing Skills; Selection of topic, thesis statement, developing the thesis; introductory, developmental, transitional and concluding paragraphs, linguistic unity, coherence and cohesion, descriptive, narrative, expository and argumentative writing.

Unit 3

Technical Writing: Scientific and technical subjects; formal and informal writings; formal writings/reports, handbooks, manuals, letters, memorandum, notices, agenda, minutes; common errors to be avoided.

SUGGESTED READINGS

1. M. Frank. Writing as thinking: *A guided process approach, Englewood Cliffs,* Prentice Hall Reagents.

2. L. Hamp-Lyons and B. Heasely: Study Writing; *A course in written English.* For academic and professional purposes, Cambridge Univ. Press.

3. R. Quirk, S. Greenbaum, G. Leech and J. Svartik: *A comprehensive grammar of the English language*, Longman, London.

4. Daniel G. Riordan & Steven A. Panley: *"Technical Report Writing Today"* - Biztaantra.

Additional Reference Books

5. Daniel G. Riordan, Steven E. Pauley, Biztantra: *Technical Report Writing Today*, 8th Edition (2004).

6. *Contemporary Business Communication*, Scot Ober, Biztantra, 5th Edition (2004).

Paper 4-MACT 101: Mathematics - I

THEORY   **Marks: 100**

Unit I: Recapitulation:

Fundamentals. Mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebric operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Mathematical series: Power series, Maclaurin, Taylor series, convergence (e.g. pressure virial equation of state, colligative properties).

Pythagoras theorem in three dimensions. Trigonometric functions, identities.

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations), differentials, higher order derivatives, discontinuities, stationary points, maximum-minimum problems, inflexion points, limiting values of functions: L'Hôpital's rule, combining limits.

Unit II: Integral calculus:

The process of integration, odd and even functions, indefinite integrals, standard integrals, methods of integration (e.g. integrated rate law for second order reaction), numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data),

probability distributions (gas kinetic theory) and mean values. Calculus of the trigonometric functions.

Calculus with several independent variables: Functions of several independent variables, change of variables, relations between partial derivatives (e.g. change in pressure for small changes in volume and temperature), total differentials, chain rules for partial differentiation, Euler's theorem, exact and inexact differentials (thermodynamics), line integrals.

Recommended Texts:

1. McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
2. Mortimer, R. *Mathematics for Physical Chemistry.* 3rd Ed. Elsevier (2005).
3. Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
4. Yates, P. *Chemical Calculations.* 2nd Ed. CRC Press (2007).

Paper 1-CHHP 101: Inorganic Chemistry - I

PRACTICAL   **Marks: 50**

   (A)   Titrimetric Analysis
 (i) Calibration and use of apparatus

         (i)   Preparation of solutions of different Molarity/Normality of titrants
(B) Acid- Base Titrations

         (i)   Estimation of carbonate and hydroxide present together in mixture.

         (ii)   Estimation of carbonate and bicarbonate present together in a mixture.

         (ii)   Estimation of free alkali present in different soaps/detergents
(C) Oxidation- Reduction Titrimetry

         (i)   Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$ solution.

         (ii)   Estimation of oxalic acid and sodium oxalate in a given mixture.

         (iii)   Estimation of Fe (II) with $K_2Cr_2O_7$ using internal (diphenylamine, anthranilic acid) and external indicator.
Reference text:

 1. Vogel, A.I. *A Textbook of Quantitative Inorganic Analysis*, ELBS.

Paper 2-CHHP 102: Organic Chemistry - I

PRACTICAL   **Marks: 50**

1. Checking the calibration of the thermometer
2. Purification of organic compounds by crystallization using the   following solvents:
    a.   Water
    b.   Alcohol
    c.   Alcohol-Water
3. Determination of the melting points of above compounds and unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
4. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds
5. Determination of boiling point of liquid compounds. (boiling point lower than and more than 100° C by distillation and capillary method)
6. Chromatography
    a.   Separation of a mixture of two amino acids by ascending and horizontal paper chromatography
    b.   Separation of a mixture of two sugars by ascending paper chromatography
    c.   Separation of a mixture of o- and p-nitrophenol or o- and p-aminophenol by thin layer chromatography (TLC

SEMESTER II

Paper 5-CHHT 203: Physical Chemistry- I

THEORY   **Marks: 100**

Unit I: Gaseous state:

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of σ from η; variation of viscosity with temperature and pressure.

Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, *Z*, and its variation with pressure for different gases. Causes of deviation from ideal behaviour. van der Waals equation of state, its derivation and application in explaining real gas behaviour, mention of other equations of state (Berthelot, Dietrici); virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states.

Unit II: Liquid state:

Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases.

Qualitative discussion of structure of water.

Unit III: Solid state:

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, 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. Defects in crystals. Glasses and liquid crystals.

Unit IV: Ionic equilibria:

Strong, moderate and weak electrolytes, 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-, di- and tri-protic acids (exact treatment).

Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry and biochemical processes in the human body.

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid – base indicators; selection of indicators and their limitations.

Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

Recommended Texts:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
2. Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).

Paper 6-CHHT 204: Analytical Methods in Chemical Analysis

THEORY   **Marks: 100**

Unit I : Qualitative and Quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q, and T test, rejection of data, and confidence intervals.

Unit II: Optical methods of analysis:

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;

Basic principle of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.

Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

Structural illustration through interpretation of data, Effect and importance of isotope substitution.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, Choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

Unit III: Thermal method of analysis:

Theory of thermogravimetry (TG), basic principle of instrumentation.

Techniques for quantitative estimation of Ca and Mg from their mixture.

Unit IV: Electro analytical methods:

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence point. Techniques used for the determination of pK_a values.

Unit V: Separation Techniques:

Solvent extraction: Classification and principle and efficiency of the technique.

Mechanism of extraction: extraction by solvation and chelation.

Technique of extraction: batch, continuous and counter current extractions.

Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and non aqueous media.

Chromatography: Classification and principle and efficiency of the technique.

Mechanism of separation: adsorption, partition & ion exchange.

Development of chromatograms: frontal, elution and displacement methods.

Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Stereo isomeric separation and analysis: Measurement of optical rotation, calculation of Enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of Enantiomeric composition using NMR, Chiral solvents and chiral shift reagents Chiral chromatographic techniques using chiral columns (GC and HPLC).

Role of computers in instrumental methods of analysis.

Recommended texts:

1. Vogel, Arthur I: *A Test book of Quantitative Inorganic Analysis* (Rev. by GH Jeffery and others) 5th Ed. The English Language Book Society of Longman
2. Willard, Hobert H. *et. al*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, Gary D; *Analytical Chemistry*, 6th Ed. New York- John Willy, 2004.
4. Harris, Daniel C: *Exploring Chemical Analysis*, 2nd Ed. New York, W.H. Freeman, 2001.
5. Khopkar, S.M. *Basic Concepts of Analytical Chemistry* New Age, International Publisher, 2009.
6. SKoog, D.A. Holler F.J. and Nieman, T.A. *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore.
7. Mikes, O. & Chalmes, R.A. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Ltd. London.
8. Ditts, R.V. *Analytical Chemistry – Methods of separation*.

Paper 7-LSPT 202-BIOLOGY-II

THEORY   **Marks: 100**

Cell and Cellular Processes

Unit 1. Techniques in Biology   **(Ch 1 Sheeler)   (12 Periods)**

Principles of microscopy; Light Microscope; Phase contrast microscopy; Fluorescence microscopy; Confocal microscopy; Sample Preparation for light microscopy; Electron microscopy (EM)- Scanning EM and Scanning Transmission EM (STEM); Sample Preparation for electron microscopy; X-ray diffraction analysis

Unit 2. Cell as a unit of Life   **(Ch 6 Campbell) (10 Periods)**

The Cell Theory; Prokaryotic and eukaryotic cells; Cell size and shape; Eukaryotic Cell components

Unit 3. Cell Organelles   **(Ch 15, 16, 17,18,19,20 Sheeler) (22 Periods)**

- **Mitochondria:**
  Structure, marker enzymes, composition; mitochondrial biogenesis; Semiautonomous organelle; Symbiont hypothesis; Proteins synthesized within mitochondria; mitochondrial DNA

- **Chloroplast**
  Structure, marker enzymes, composition; semiautonomous nature, chloroplast DNA

- **ER, Golgi body & Lysosomes**
  Structures and roles. Signal peptide hypothesis, N-linked glycosylation, Role of golgi in O-linked glycosylation. Cell secretion, Lysosome formation.

- **Peroxisomes and Glyoxisomes:**
  Structures, composition, functions in animals and plants and biogenesis

- **Nucleus:**
  Nuclear Envelope- structure of nuclear pore complex; chromatin; molecular organization, DNA packaging in eukaryotes, euchromatin and heterochromatin, nucleolus and ribosome structure (brief).

Unit 4. Cell Membrane and Cell Wall   **(Ch 7 Campbell / Ch 15 Sheeler / Ch 3 Raven)**

The functions of membranes; Models of membrane structure; The fluidity of membranes; Membrane proteins and their functions; Carbohydrates in the membrane; Faces of the membranes; Selective permeability of the membranes; Cell wall

Unit 5. Cell Cycle: Interphase, Mitosis and Meiosis   (Ch 12, 13 Campbell) (8 Periods)

Role of Cell division; Overview of Cell cycle; Molecular controls; Meiosis

SUGGESTED BOOKS

1. Campbell, N.A. and Reece, J. B. (2008) Biology 8th edition, Pearson Benjamin Cummings, San Francisco.

2. Raven, P.H et al (2006) Biology 7th edition Tata McGrawHill Publications, New Delhi

3. Sheeler, P and Bianchi, D.E. (2006) Cell and Molecular Biology, 3rd edition, John Wiley & sons NY

Paper 8-PHCT 201: Physics-I

THEORY   **Marks: 100**

Unit I :Mathematical Physics: Scalar and vector products, polar and axial vectors, triple and quadruple products.

Unit II:Vector calculus:

Scalar and vector fields, differentiation of a vector, gradient, divergence, curl and Δ operations and their meaning, idea of line, surface and volume integrals, Gauss and Stokes' theorem.

Unit III: Classical Mechanics:

Particle dynamics: Newton's laws of motion, conservation of linear momentum, centre of mass, conservative forces, work energy theorem, particle collision.

Rotational kinematics and dynamics: Rotational motion, forces and pseudo forces, torque and angular momentum, kinetic energy of rotation, rigid body rotation dynamics, moment of inertia, conservation of angular momentum, comparison of linear and angular momentum, motion of a top.

Oscillations: Linearity and superposition principle, free oscillation with one and two degrees of freedom, simple pendulum, combination of two simple harmonic motions.

Lissajous figures, free and damped vibrations, forced vibrations and resonance, Q factor, wave equation, travelling and standing waves, superposition of waves, phase and group velocity.

Unit IV :Wave optics: Interference, division of amplitudes, Young's double split, Fresnel's biprism, interference in thin films and wedged shaped films.

Fresnel diffraction: Diffraction at a single slit and a circular aperture, diffraction at a double split, plane transmission grating, resolving power of a telescope and a microscope, resolving and dispersive power of a plane diffraction grating.

Polarization: Polarization by reflection and refraction, Brewster's law, double refraction, nicol prism, quarter and half-wave plates, Production and analysis of circularly and elliptically polarized light.

Recommended Texts:

1. Spiegel, M. R. *Vector Analysis* Schaum's Outline Series. McGraw-Hill Book Co.: Singapore (1974)
2. Beiser, A. *Concepts of Modern Physics* McGraw-Hill Education (2002).
3. Resnick, R., Halliday, D. & Krane, K. S. Physics Vol. I and II 5th Ed. John Wiley & Sons (2004)
4. Serway, R. A. & Jewett, J. W. *Physics for Scientists and Engineers* 6th Ed.

Paper 5-CHHP 203: Physical Chemistry - I

PRACTICAL   **Marks: 50**

(I) **Surface tension measurements** (use of organic solvents excluded).
   a) Determine the surface tension by (i) drop number (ii) drop weight method.
   b) Study the variation of surface tension of detergent solutions with concentration
(II) **Viscosity measurement using Ostwald's viscometer** (use of organic solvents

excluded).

(a) Study the effect of the addition of solutes such as (i) polymer (ii) ethanol (iii) sodium chloride on the viscosity of water at room temperature.

(b) Study the effect of variation of viscosity of an aqueous solution with the concentration of solute.

(III) **pH measurements**

b) Measurement of pH of different solutions using pH-meter.

c) Preparation of buffer solutions
        (i) Sodium acetate-acetic acid
        (ii) Ammonium chloride-ammonium hydroxide

Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

d) pH metric titrations of
        (i) strong acid and strong base
        (ii) weak acid and strong base

Any other experiment carried out in the class.

Paper 6-CHHP 204: Analytical Methods in Chemical Analysis

PRACTICAL   **Marks: 50**

Separation Techniques

1.   Chromatography:

(a) Separation of mixtures

    (i)   Paper chromatographic separation of Fe^{3+}, Al^{3+}, and Cr^{3+}

        (ii)   Separate and identify the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography.

            Report the R_f values.

(b) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their R_f values.

(c) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

2. Solvent Extractions:
    (i) To separate a mixture of Ni^{2+} & Fe^{3+} by complexing with DMG and extracting

the Ni^{2+} DMG complex in chloroform, and determine its concentration with spectrophotometry.

(ii) Solvent extraction of zisconium with amberliti LA-1, separation from a mixture of irons and gallium.

3. Determine the pH of given aerated drinks fruit juices, shampoos and soaps.

4. Determination of Na, Ca, Li in cola drinks and fruit juices using fame photometric techniques.

5. Analysis of soil:

   (i) Determination of pH of soil.

   (ii) Total soluble salt

   (iii) Estimation of calcium, magnesium, phosphate, nitrate

6. Ion exchange:

   (i) Determination of exchange capacity of cation exchange resins and anion exchange resins.

   (ii) Separation of metal ions from their binary mixture.

   (iii) Separation of amino acids from organic acids by ion exchange chromatography.

7. Determination of pK_a values of indicator using spectrophotometry.

8. Structural characterization of compounds by Infra-Red spectroscopy.

9. Determination of dissolved oxygen in water.

10. Determination of chemical oxygen demand (COD).

11. Determination of Biological oxygen demand (BOD).

Paper 7- LSPP 202-BIOLOGY-II

PRACTICALS   **Marks: 50**

1. To study prokaryotic cells (bacteria), viruses, eukaryotic cells with the help of light and electron micrographs.
2. Study of the photomicrographs of cell organelles
3. To study the structure of plant cell through temporary mounts.
4. To study the structure of animal cells by temporary mounts-squamous epithelial cell and nerve cell.
5. Preparation of temporary mounts of striated muscle fiber
6. To prepare temporary stained preparation of mitochondria from striated muscle cells /cheek epithelial cells using vital stain Janus green.
7. To prepare temporary stained squash from root tips of *Allium cepa* and to study the various stages of mitosis.
8. Study the effect of temperature, organic solvent on semi permeable membrane.
9. Demonstration of dialysis of starch and simple sugar.
10. Study of plasmolysis and deplasmolysis on *Rhoeo* leaf.
11. Measure the cell size (either length or breadth/diameter) by micrometry.
12. Study the structure of nuclear pore complex by photograph (from Gerald Karp)

Paper 8- PHCP 201-PHYSICS-I

PRACTICALS   **Marks: 50**

Each student is expected to do at least 3 experiments each from Group A and Group B.

Group A experiments

A-1. Determination of spring constant of a spring by (i) static, and (ii) dynamic methods.

A-2. Study of damped harmonic oscillator- Q factor.

A-3. Determination of temperature coefficient of resistance using platinum resistance thermometer.

A-4. Study of thermal couple calibration and inversion temperature.

A-5. LCR study of resonance Q-factor.

A-6. Kator's pendulum- Bar pendulum.

Group B experiments

B-1. Determination of wavelength of light by Fresnel's biprism.

B-2. Determination of wavelength of sodium light by Newton's arrangement.

B-3. Determination of refractive index of tint glass using a spectrometer.

B-4. Determination of dispersive power of a glass prism using Cauchy's constant. Also determine the resolving power of a prism.

B-5. Determination of wavelength of sodium light using a plane transmission grating and resolving power of a diffraction grating.

B-6. Determination of specific rotation of cane sugar solution using a polarimeter.

<u>SEMESTER – III</u>

Paper 9-CHHT 305: Inorganic Chemistry -II

THEORY   **Marks: 100**

Unit I: Chemical Bonding:

(i)   Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy.

(ii)   Covalent bond: Lewis structure, Valence Bond theory (Heitler-London approach). Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2, O_2, C_2, B_2, F_2, CO, NO, and their ions; HCl, BeF_2, CO_2, (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach), and bond lengths.

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(iii) Metallic Bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.
(iv) Weak Chemical forces: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Hydrogen bonding (theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points, solubility energetics of dissolution process.
(v) Acids and Bases: Brönsted- Lowry concept of acid-base reaction, solvated proton, relative strength of acids, types of acid-base reactions, levelling solvents, Lewis acid-base concept, Classification of Lewis acids, Hard and Soft Acids and Bases (HSAB) Application of HSAB principle.

Recommended Texts:

1. Huheey, J.E. *Inorganic Chemistry*, Prentice Hall 1993

2. Douglas, B.E. and Mc Daniel, D.H., *Concepts & Models of Inorganic Chemistry*, Oxford 1970

3. Lee, J.D. *Concise Inorganic Chemistry*, ELBS (1991)
4. Shriver & Atkins, *Inorganic Chemistry*, Third Edition, Oxford Press 1994.
5. H.W. Porterfield, *Inorganic Chemistry,* Second Edition, Academic Press, 2005.

Paper 10-CHHT 306: Organic Chemistry -II

THEORY   **Marks: 100**

Unit I: Chemistry of Halogenated hydrocarbons:

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

Aryl halides: Preparation, including preparation from diazonium salts. nucleophilic aromatic substitution; S_NAr, Benzyne mechanism

Relative reactivity of Alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Organometallic compounds of Mg and Li – Use in synthesis of organic compounds.

Unit II: Alchols, Phenols, Ethers and epoxide:

Alcohols: preparation, properties and relative reactivity of 1^0, 2^0, 3^0 alcohols, Bouvaelt-Blanc Reduction; Preparation and properties of glycols: Oxidation by periodic acid and lead tetraacetate, Pinacol- Pinacolone rearrangement;

Phenols: Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer – Tiemann and Kolbe's – Schmidt Reactions, Fries and Claisen rearrangements with mechanism;

Ethers and Epoxides: Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and $LiAlH_4$

Unit III: Carbonyl Compounds:

Structure, reactivity and preparation;

Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisan-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 and PGC);

Addition reactions of unsaturated carbonyl compounds: Michael addition.

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

Unit IV:Carboxylic Acids and their Derivatives:

Preparation, physical properties and reactions of monocarboxylic acids:

Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids;

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic sustitution at acyl group - Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann-bromamide degradation and Curtius rearrangement

Unit V: Sulphur containing compounds:

Preparation and reactions of thiols, thioethers and sulphonic acids.

Recommended Texts:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

 2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Paper 11-CHHT 307: Physical Chemistry -II

THEORY **Marks: 100**

Unit I : Chemical thermodynamics:

Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.

First law: Concept of heat, q, work, w, internal energy U and statement of first law; enthalpy, H, relation between heat capacities, calculations of q, w, U and H for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions.

Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond

dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature.

Second Law: Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics; molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes.

Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules.

Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity. Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

Unit II : Systems of variable composition:

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

Unit III: Chemical equilibrium:

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants K_p, K_c and K_x. Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Unit IV: Solutions and colligative properties:

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions.

Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

Recommended Texts:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
2. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
3. Engel, T. & Reid, P. *Thermodynamics, Statistical Thermodynamics, & Kinetics* Pearson Education, Inc: New Delhi (2007).
4. McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi (2004).

Paper 12-MACT 302: Mathematics - II

THEORY   **Marks: 100**

Differential equations: differential equations with separable variables, series solution, numerical solutions of differential equations. Newton' laws of motion. The linear harmonic oscillator: Linear differential equations with constant coefficients.

Partial differential equations: separation of variables. The wave equation. Schrödinger's equation.

Multiple integrals. Changing variables. Vector derivative operators. Multiple integrals involving other coordinate systems (spherical polar). Maximum and minimum values of functions of several variables.

Stationary points, imaginary and complex numbers, complex plane, Euler's formula and polar form of complex numbers, complex conjugates, modulus of a complex number.

Operators: operator algebra, linear operators, eigenfunctions and eigenvalues, commutators of operators, Hermitian operators.

Vectors and coordinate systems: Unit vectors (application in solid state), addition and subtraction of vectors, multiplication of vectors. Vector calculus. Vectors and coordinate systems in three dimensions (Cartesian, spherical polar and their interconversion).

Determinants. Matrix algebra, Simultaneous equations: method of substitution and elimination, consistency and independence. Homogeneous linear equations. Simultaneous equations with more than two unknowns (e.g. spectrophotometry), Cramer's rule, matrix inversion, orthogonal and unitary matrices, matrix eigenvalues and eigenvectors, diagonalization of a matrix.

Recommended Texts:

1. McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
2. Mortimer, R. *Mathematics for Physical Chemistry.* 3rd Ed. Elsevier (2005).
3. Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
4. Yates, P. *Chemical calculations.* 2nd Ed. CRC Press (2007).

Paper 9-CHHP 305: Inorganic Chemistry -II

PRACTICAL   **Marks: 50**

(a) Iodo / Iodimetric Titrations

        (i)   Estimation of Cu (II) and $K_2Cr_2O_7$ Using sodium thiosulphate

                    solution (Iodimetrically).

        (ii)   Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically

        (iii)   Estimation of available chlorine in bleaching powder iodometrically.

(b) Inorganic preparations

  (i) Cuprous Chloride, Cu_2Cl_2

  (ii) Preparation of Manganese (III) phosphate, $MnPO_4.H_2O$

        (iii)   Preparation of Aluminium Potassium sulphate $KAl(SO_4)_2.12H_2O$ (Potash alum) or Chrome alum.

Recommended Texts:

1. Vogel, A.I. A text book of quantitative Inorganic Analysis, ELBS. 1978.

Paper 10-CHHP 306: Organic Chemistry -II

PRACTICAL   **Marks: 50**

Organic preparations

1. Acetylation of one of the following compounds: amines (aniline, o-,m- ,p- toluidines and o-,m-,p- anisidine) and phenols (β-naphthol, vanillin, salicylic acid)
2. Benzolyation of one of the following compounds: amines (aniline, o-,m-,p- toluidines and o-,m-,p- anisidine) and phenols (β-naphthol, resorcinol, p-cresol) by Schotten-Baumann reaction
3. Hydrolysis of amides and esters to obtain benzoic acid
4. Derivatives of the carbonyl compounds:
   ➢ 2,4-DNP of one the following compounds- acetone, ethyl methyl ketone, di-ethyl ketone, cyclohexanone
   ➢ semicarbazone of one the following compounds- acetone, ethyl methyl ketone, di-ethyl ketone, cyclohexanone
   ➢ oxime of one the following compounds- di-ethyl ketone, cyclohexanone
5. Nitration of one the following compounds: nitrobenzene, chlorobenzene, bromobenzene
6. Oxidation of the following compounds: benzaldehyde, benzyl alcohol acetophenone to benzoic acid (by iodoform reaction)

The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may used for recrystallization, melting point etc.

Paper 11-CHHP 307: Physical Chemistry -II

PRACTICAL   **Marks: 50**

(I) **Thermochemistry**
   (a) Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).
   (b) Determination of heat capacity of the calorimeter and enthalpy of neutralization of

hydrochloric acid with sodium hydroxide.

(c) Calculation of the enthalpy of ionization of ethanoic acid.

(d) Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.

(e) Determination of basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.

(f) Determination of enthalpy of hydration of copper sulphate.

(g) Study of the solubility of benzoic acid in water and determination of ΔH.

(II) Indexing of given powder diffraction pattern of a cubic crystalline system.

Any other experiment carried out in the class.

<u>SEMESTER IV</u>

Paper 13-CHHT 408: Inorganic Chemistry -III

THEORY   **Marks: 100**

Unit I : Chemistry of *s* and *p* block elements:

Inert pair effect, Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Complex formation tendency of *s* and *p* block elements.

Hydrides and their classification ionic, covalent and interstitial. Basic beryllium acetate and nitrate.

Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses.

Boric acid and borates, boron nitrides, borohydrides (diborane) carboranes and graphitic compounds, silanes, Oxides and oxoacids of nitrogen, Phosphorus and chlorine. Peroxo acids of sulphur, interhalogen compounds, polyhalide ions, pseudohalogens and basic properties of halogens.

Theoretical principles involved in volumetric analysis, done in the lab.

Unit II : Noble gases :

Occurrence & uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF_2 and XeF_4, XeF_6; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF_2). Molecular shapes of noble gas compounds (VSEPR theory).

Unit III : Inorganic Polymers:

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates and phosphazenes, and polysulphates.

Recommended Texts:

1. Greenwood, N.N. and Earnshaw, *Chemistry of the Elements*, Butterworth-Heinemann. 1997.
2. Lee, J.D. *Concise Inorganic Chemistry*, ELBS (1991).
3. Canham, G.R. and Overton, T., *Descriptive Inorganic Chemistry*, Freeman & Co.2006
4. Cotton, F.A. and Wilkinson, G, *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.

Paper 14-CHHT 409: Organic Chemistry -III

THEORY   **Marks: 100**

Unit I: Nitrogen Containing Functional Groups

Preparation and important reactions of nitro and compounds, nitriles and isonitriles

Amines: Effect of substituent and solvent on basicity; Preparation and properties: Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction; Distinction between 1^0, 2^0 and 3^0 amines with Hinsberg reagent and nitrous acid;

Diazonium Salts: Preparation and their synthetic applications.

Unit II: Polynuclear Hydrocarbons

Reactions of naphthalene phenanthrene and anthracene Structure, Preparation and structure elucidation and important derivatives of naphthalene and anthracene; Polynuclear hydrocarbons.

Unit III: Heterocyclic Compounds

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine, Structure elucidation of indole, Fischer indole synthesis and Madelung synthesis), Structure elucidation of quinoline and isoquinoline, Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction

Derivatives of furan: Furfural and furoic acid.

Unit IV: Alkaloids

Natural occurrence, General structural features, Isolation and their physiological action

Hoffmann's exhaustive methylation, Emde's modification, Structure elucidation and synthesis of Hygrine and Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine.

Recommended Texts:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, 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: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Paper 15-CHHT 410: Physical Chemistry -III

THEORY   **Marks: 100**

Unit I: Phase equilibria

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for non-reactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications.

Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions.

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

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and nonideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation.

Nernst distribution law: its derivation and applications.

Unit II: Electrochemistry

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry.

Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining   (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb_2O_3 electrodes. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation).

Recommended Texts:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
2. Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).

Paper 16-PHCT 402: Physics-II

THEORY   **Marks: 100**

Unit I: Electrostatics:

Electric field, potential due to a charge distribution and due to a dipole, electrical potential energy, flux, Gauss's law, electric field in a dielectric, polarization, energy stored in an electric field.

Unit II : Magnetism:

Magnetic field due to a current-carrying conductor, Biot Savart law, magnetic force on a current, Lorentz force, electromagnetic induction, Lenz's law, magnetic properties of matter, para- dia- and ferromagnetism, spinning of a magnetic dipole in an external magnetic field.

Unit III: Fundamental laws of electromagnetism:

Modification of Ampere's law, equation of continuity and displacement current, Maxwell's equations, wave equation and its plane wave solution, nature of electromagnetic waves, tranversality and polarization, propagation of electromagnetic plane waves in dielectric media.

Unit IV : Electronics:

Half-wave, full-wave and bridge rectifiers, ripple factor, rectification efficiency, filters (series in inductor, shunt capacitor, LC and π sections), voltage regulations, load regulation, Zener diode as voltage regulator. Characteristic curves of bipolar

transistors, static and dynamic load line, biasing (fixed and self) of transistor circuit, thermal instability of bias, the black box idea of CE, CB and CC transistor circuits as two-port network, small signal active output, hybrid model of a CE transistor circuit, analysis of a small signal amplifier: its voltage and current gains, negative and positive feedback. Barkhausen's criterion for self-sustaining oscillations, LC and phase shift oscillators.

Unit V: Digital electronics:

Number systems (binary, BCD, octal and hexadecimal), 1's and 2's complements. Logic gates, AND, OR, NAND, NOR, XOR and NXOR. Boolean algebra (Boolean laws and simple expressions), binary adders, half adder, half subtractor, full adder and full subtractor.

Recommended Texts:

1. Griffiths, D. J. *Introduction to Electromagnetism* 3rd Ed. Prentice-Hall (1999).
2. Malvino, A.P. & Leach, D. P. *Digital Principles and Applications*, Tata McGraw-Hill (2008).
3. Ryder, J. D. *Electronic Fundamentals and Applications: Integrated and Discrete Systems.* 5th Ed. Prentice-Hall, Inc. (2007).
4. Floyd, T. L. & Buchla, D. M. *Electronics Fundamentals: Circuits, Devices and Applications* (8th Ed.) Prentice-Hall (2009).

Paper 13-CHHP 408: Inorganic Chemistry -III

PRACTICAL   **Marks: 50**

(a) Complexometric Titrations:

    (i)   Complexometric estimation of (i) Mg^{2+} (ii) Zn^{2+} using EDTA

    (ii)   Estimation of total hardnesss of water samples

    (iii)   Estimation of Ca^{2+} in solution by (substitution method) using Erio-chrome black-T as indicator.

    (ii)   Estimation of Ca/Mg in drugs and Biological samples.

(b) **Argentometry**
Estimation of Cl^- (i) By Mohr's method, (ii) By Vohlard's method, (iii) By Fajan's method.

(c) Paper Chromatographic separation of Ni (II) and Co(II); Cu(II) and Cd (II)C

Paper 14-CHHP 409: Organic Chemistry -III

PRACTICAL **Marks: 50**

Organic Preparations

1. Diels-Alder reaction between anthracene and maleic anhydride
2. Reduction: nitrobenzene to azobenzene (TLC of the mixture), m-dinitrobenzene to m-nitroaniline
3. S-benzylisothiuranum salts of any one water soluble and one water insoluble acid: acetic acid, phenyl acetic acid, oxalic acid, benzoic acid, phthalic acid
4. Photochemical reduction of benzophenone to benzopinacol
5. Benzoin condensation of benzaldehyde (using thiamine hydrochloride)
6. Condensation of p-toluidine with benzaldehyde/salicylaldehyde/2-hydroxy-3-methoxy benzadehyde to get Schiff's base (solventless condensation)

Estimation of:

1. Phenol and aniline by bromination with potassium bromate-potassium bromide method
2. Glycine by formylation method
3. Saponification value of an oil/fat

Paper 15-CHHP 410: Physical Chemistry -III

PRACTICAL **Marks: 50**

(I) Study the equilibrium of at least one of the following reactions by the distribution method:

(i) $I_2(aq) + I^- \rightarrow I_3^- (aq)$

(ii) $Cu^{2+}(aq) + nNH_3 \rightarrow Cu(NH_3)_n^{2+}$

(II) Perform the following potentiometric titrations (at least two):

(i) Strong acid with strong base (ii) weak acid with strong base and (iii) dibasic acid with strong base

(III) Potentiometric titration of Mohr's salt with potassium dichromate.

(IV) Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.

(V) Phase equilibria: Construction of the phase diagram of (i) simple eutectic and (ii) congruently melting systems, using cooling curves and ignition tube methods.

Any other experiment carried out in the class.

Paper 16-PHCP 402: Physics-II

PRACTICAL   **Marks: 50**

1. Study of a Ballistic Galvanometer: resistance, current sensitivity, charge   sensitivity, and critical damping resistance of the galvanometer.

2. Determination of high resistance by leakage method.

3. Determination of mutual inductance by Ballistic Galvanometer.

4. Operations and measurements by Cathode Ray Oscilloscope (CRO). Calibration of DC and AC voltages, frequency and phase measurements of a signal.

5. Study of transistor characeteristics (CB, CE, CC configurations).

6. Study of power supply (rectification factor, voltage and load regulation for   C, L, CL and π filters).

7. Study of basic RC coupled amplifier (frequency response and band width).

8. Study of Colpitts oscillator.

9. Self-inductance measurement by Owen's bridge.

10. Measurement of magnetic field by search coil.

11. To verify experimentally OR, NAD, NOT, NOR, NAND gates.

12. Study of Half-Adder/ Subtractor.

Paper 17-CHHT 511: Inorganic Chemistry -IV

THEORY   **Marks: 100**

Unit I : Coordination Chemistry

Werner's theory, valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (Δo), CFSE in weak and strong fields, pairing energies, factors effecting the magnitude of 10 Dq (Δo, Δt). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory.

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Chelate effect, polynuclear complexes, Labile and inert complexes.

Unit II: Transition elements: General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer & Bsworth diagrams). Difference between the first, second and third transition series.

Chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states (excluding their metallurgy)

Unit III: Lanthanoids and actinoids: electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only).

Recommended Texts:

1. Purecell, K.F. and Kotz, J.C., *Inorganic Chemistry* W.B. Saunders Co. 1977.
2. Basolo, F, and Pearson, R.C., *Mechanisms of Inorganic Chemistry*, John Wiley & Sons, NY, 1967.
3. Greenwood, N.N. & Earnshaw A., *Chemistry of the Elements*, Butterworth-Heinemann,1997.

Paper 18-CHHT 512: Organic Chemistry -IV

THEORY **Marks: 100**

Unit I: Carbohydrates

Occurrence, classification and their biological importance

Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures; Interconversions of aldoses and ketoses; Killiani-Fischer synthesis and Ruff degradation;

Disaccharides – Structure elucidation of maltose, lactose and sucrose

Polysaccharides – Elementary treatment of starch, cellulose and glycogen.

Unit II: Nucleic Acids

Components of nucleic acids, Nucleosides and nucleotides;

Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil nd Thymine; Structure of polynucleotides.

Unit III: Amino acids, Peptides and Proteins

Amino acids, Peptides and their classification.

α-Amino Acids - Synthesis, ionic properties and reactions. Zwitterions, pK_a values, isoelectric point and electrophoresis;

Study of peptides: determination of their primary structures-end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups - Solid-phase synthesis

Unit IV: Lipids

Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenntion of fats and oils, Saponification value, acid value, iodine number. Reversion and rancidity.

Unit V: Pharmaceutical Compounds: Structure and Importance

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis).

An elementary treatment of Antibiotics and detailed study of chloramphenicol,

Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine)

Unit VI: Terpenes

Occurrence, classification, isoprene rule; Elucidation of stucture and synthesis of Citral, Neral and α- terpineol.

Recommended Texts:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, 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: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

4. Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Bioch*emistry, Fourth Edition, W. H. Freeman.

5. Berg, J. M., Tymoczko, J. L. & Stryer, L. *Biochemistry*, Sixth Edition, W. H. Freeman.

Paper 19-CHHT 513: Physical Chemistry -IV

THEORY   **Marks: 100**

Unit I : Conductance

Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and 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, and (v) hydrolysis constants of salts.

Unit II: Chemical Kinetics

Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions   (ii) parallel reactions   and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms)   (iv) chain reactions.

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates.

Surface chemistry: Physical adsorption, chemisorption, adsorption isotherms. nature of adsorbed state.

Catalysis: Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis.

Unit III: Photochemistry

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws, of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence.

Recommended Texts:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
2. Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. Laidler, K. J. *Chemical Kinetics* Pearson Education: New Delhi (2004).

Paper 20-CHHT 514: Biochemistry and Environmental Chemistry

THEORY   **Marks: 100**

Unit I:

   Carbohydrates: Biological importance of carbohydrates, Metabolism, Cellular currency of energy (ATP), Glycolysis, Alcoholic and Lactic acid fermentations,Krebs cycle

   Proteins: classification, biological importance; Primary, secondary and tertiary structures of proteins: α-helix and β- pleated sheets, Denaturation of proteins

   Enzymes: Nomenclature, Characteristics (mention of Ribozymes), Classification;Active site, Mechanism of enzyme action, Stereospecificity of enzymes,Coenzymes and cofactors, Enzyme inhibitors, Introduction to Biocatalysis:Importance in "Green Chemistry" and Chemical Industry

Unit II:

   Lipids: Biological importance of triglycerides and phosphoglycerides and cholesterol; Lipid membrane, Liposomes and their biological functions and underlying applications.

   Structure of DNA (Watson-Crick model) and RNA, Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation, Introduction to Gene therapy.

Unit III:

Environment and it's segments, Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulfur

Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical Smog: its constituents and photochemistry, Environmental effects of Ozone, Major sources of Air pollution

Effects of air pollution on living organisms and vegetation, Controls of air pollution, Climate change, Green house effect, global warming. Techniques of measuring air pollutants.

Water Pollution: Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems. Water purification methods

Unit IV:

Energy and Enviornment: Sources of energy: Coal, petrol and Natural gas. Nuclear Fusion / Fisson, Solar energy, Hydrogen, geothermal, Tidal and Hydel etc.

Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and it's Management

Recommended Texts:
1. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) Biochemistry. VI the Edition. W.H. Freeman and Co.
2. Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) principles of Biochemistry.IV Edition. W.H. Freeman and Co.
3. Murray, R.K., Granner, D.K., Mayes, P.A. and Rodwell, V.W. (2009) Harper's Illustrated Biochemistry. XXVIII edition. Lange medical Books/ McGraw-Hill
4. Manahan S.E. (2005) Environmental Chemistry, CRC Press
5. Miller, G.T. (2006) Environmental Science 11th edition. Brooks/Cole
6. Mishra, A. (2005) Environmental Studies. Selective and Scientific Books, New

Paper 17-CHHP 511: Inorganic Chemistry -IV

PRACTICAL   **Marks: 50**

   (a)   Quantitative Analysis: The following quantitative estimations are to be carried out.

   (i)   Estimation of nickel (II) using Dimethylglyoxime as the precipitant.

(ii)   Estimation of copper as CuSCN

(iii)   Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$ through (i) Heterogeneous and (ii) Homogeneous media.

(iv)   Estimation of Al (III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminium oxinate).

    (b)   Inorganic Preparations

        (i)   Tetraammine copper (II) sulphate, $[Cu(NH_3)_4]SO_4 H_2O$

        (ii)   Potassium trisoxalatochromate (III), $K_3[Cr(C_2O_4)_3]$

        (iii)   Cis and trans $K[Cr(C_2O_4)_2 (H_2O_2]$ Potassium dioxalatodiaquachromate (III)

        (iv)   Pentaammine carbonato Cobalt (III) ion

    (c)   Spectrophotometric estimation of Ferrous ions by using 1,10 phenanthroline

Recommended Texts:

1. Vogel, A.I. A text book of Quantitative Analysis, ELBS 1986.

Paper 18-CHHP 512: Organic Chemistry -IV

PRACTICAL   **Marks: 50**

1. Systematic analysis of extra elements in the given unknown compounds

2. Tests for following functional groups and unsaturation

3. Qualitative analysis of the following types of unknown organic compounds

        ➢   Carboxylic acids
        ➢   Phenols
        ➢   Alcohols
        ➢   Aldehydes
        ➢   Ketones
        ➢   Esters

Paper 19-CHHP 513: Physical Chemistry -IV

PRACTICAL   **Marks: 50**

   (I)   To study changes in conductance in the following systems
           (i) strong acid-strong base

           (ii) weak acid-strong base and
           (iii) mixture of strong acid and weak acid-strong base
   (II)   Study the kinetics of the following reactions.
              1. Initial rate method: Iodide-persulphate reaction
              2. Integrated rate method:
         (a) Acid hydrolysis of methyl acetate with hydrochloric acid, volumetrically or conductometrically.
         (b) Iodide-persulphate reaction
         (c) Saponification of ethyl acetate.

Any other experiment carried out in the class.

Paper 20-CHHP 514: Biochemistry and Environmental Chemistry

PRACTICAL   **Marks: 50**

1. To perform quantitative estimation of protein using Lowry's method. Determine

the concentration of the unknown sample using the standard curve plotted.

2. Study of the action of salivary amylase at optimum conditions

3. Effect of pH on the action of salivary amylase

4. Effect of temperature on the action of salivary amylase

5. Effect of inhibitor on the action of salivary amylase

6. Study of the activity of Trypsin using fresh tissue extracts.

7. To study the effect of temperature, organic solvents, on semi-permeable

membrane.

8. Isolation of Genomic DNA from E Coli

9. Qualitative analysis of the soil from different locations for pH and different

water soluble cations and anions

10. Quantitative estimation of oxidisable organic matter in soil, carbonate and bicarbonates by volumetry and calcium and magnesium by EDTA titration.

11. Hardness of water by EDTA titration

12. Study of pH and conductivity of tap water and polluted water.

SEMESTER VI

Paper 21-CHHT 615: Inorganic Chemistry -V

THEORY   **Marks: 100**

Unit I: Theoretical principles:

Theoretical principles and chemistry involved in qualitative analysis of mixture of cations and anions including interfering and insolubles.

Unit II: Organometallic Compounds:

Definition and classification of organometallic compounds, EAN rule.

Unit III: Metal carbonyls:

Preparation, properties, structure and bonding of mononuclear carbonyls. π-acceptor behaviour of carbon monoxide, synergic effect (MO diagram of CO) Carbonylate anions, ferrocene and its reactions.

Unit IV: Bioinorganic Chemistry:

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine.

Iron and its application in bio-systems, Hemoglobin; Storage and transfer of iron.

Recommended Texts:

1. Purcell, K.F & Kotz, J.C. *Inorganic Chemistry* W.B. Saunders Co, 1977.
2. Huheey, J.E., *Inorganic Chemistry*, Prentice Hall, 1993.
3. Lippard, S.J. & Berg, J.M. *Principles of Bioinorganic Chemistry* Panima Publishing Company 1994.
4. Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry*. Wiley-VCH, 1999.

Paper 22-CHHT 616: Organic Chemistry -V

THEORY   **Marks: 100**

Unit I: Organic spectroscopy

General principles Introduction to absorption and emission spectroscopy.

UV Spectroscopy: Types of electronic transitions, λ_{max}, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of λ_{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; IR absorption positions of O, N and S containing functional groups; Effect of H- bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin – Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpetation of NMR spectra of simple compounds

Applications of IR, UV and NMR for identification of simple organic molecules.

Unit II: Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing;

Synthesis and applications of: Azo dyes – Methyl Orange and Congo Red (mechanism of Diazo Coupling); Triphenyl Methane Dyes - Malachite Green, Rosaniline and Crystal Violet; Phthalein Dyes – Phenolphthalein and Fluorescein;

Natural dyes –structure elucidation and synthesis of Alizarin and Indigotin;

Edible Dyes with examples.

Unit III: Polymers

Introduction and classification including di-block, tri-block and amphiphilic polymers; Number average molecular weight, Weight average molecular weight, Degree of polymerization, Polydispersity Index.

Polymerisation reactions - Addition and condensation - Mechanism of cationic, anionic and free radical addition polymerization; Metallocene-based Ziegler-Natta polymerisation of alkenes;

Preparation and applications of plastics – thermosetting (phenol-formaldehyde, Polyurethanes) and thermosoftening (PVC, polythene);

Fabrics – natural and synthetic (acrylic, polyamido, polyester);

Rubbers – natural and synthetic: Buna-S, Chloroprene and Neoprene; Vulcanization;

Polymer additives; Introduction to liquid crystal polymers;

Biodegradable and conducting polymers with examples.

Recommended Texts:

1. Kemp, W. *Organic Spectroscopy*, Palgrave.

    2. Kalsi, P. S. *Textbook of Organic Chemistry* (1st Ed.), New Age International (P) Ltd. Pub.

    3. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

    4. Billmeyer, F. W. *Textbook of Polymer Science*, John Wiley & Sons, Inc.

5. Gowariker, V. R., Viswanathan, N. V. & Sreedhar, J. *Polymer Science*, New Age International (P) Ltd. Pub.

Paper 23-CHHT 617: Physical Chemistry -V

THEORY   **Marks: 100**

Unit I: Quantum Chemistry

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wavefunctions, probability distribution functions, nodal properties, Extension to two and three dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component.

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression), radial distribution functions of $1s$, $2s$, $2p$, $3s$, $3p$ and $3d$ orbitals. Average and most probable distances of electron from nucleus.

Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+. Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H_2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for

MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic (BeH_2, H_2O) molecules. Qualitative MO theory and its application to AH_2 type molecules. Simple Hückel Molecular Orbital (HMO) theory and its application to simple polyenes (ethene, butadiene).

Unit II: Molecular Spectroscopy:

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.

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, P, Q, R branches.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules.

Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

Recommended Texts:

1. Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4th Ed. Tata McGraw-Hill: New Delhi (2006).
2. Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill (2001).
3. House, J. E. *Fundamentals of Quantum Chemistry* 2nd Ed. Elsevier: USA (2004).

4. Lowe, J. P. & Peterson, K. *Quantum Chemistry* Academic Press (2005).

Paper 24-CHHT 618: Applications of Computers in Chemistry

THEORY **Marks: 100**

Unit I :Recapitulation of computer basics:

PC hardware, operating systems, data storage and backup, networks, information technology. Basic operations using windows.

Unit II: Computer programming:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

BASIC programs for numerical differentiation and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method), numerical solution of differential equations.

Conceptual background of molecular modelling: Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

Recommended Texts:

1. Noggle, J. H. *Physical chemistry on a Microcomputer.* Little Brown & Co. (1985).
2. Venit, S.M. *Programming in Basic: Problem solving with structure and style.* Jaico Publishing House: Delhi (1996).
3. Engel, T. & Reid, P. *Physical Chemistry* 2nd Ed. Pearson (2010). Chapter on Computational Chemistry.

Paper 21-CHHP 615: Inorganic Chemistry -V

PRACTICAL   **Marks: 50**

Qualitative analysis:

Using H_2S /PTC/ Thioacetamide or any other reagent. Identification of cations and simple anions in a mixture of salts containing not more than six ions (Three cations and three anions) interfering anions using semimicro scheme of analysis. If combination of cations or anions is given in the mixture, insoluble should be avoided. Spot tests should be carried out for final identifications wherever feasible.

Cation : Pb^{2+}, Bi^{3+} Cu^{2+}, Cd^{2+}, As^{3+}, Sb^{3+}, Sn^{2+} or Sn^{4+}, Fe^{2+} OR Fe^{3+}, Al^{3+}, Cr^{3+}, Co^{2+}, Ni^{2+}, Zn^{2+}, Mn^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}, NH_4^+, K^+

Anion : CO_3^{2-}, SO_3^{2-}, CO_3^2, SO_3^{2-}, S^{2-}, NO_2^-, $CH_3 COO^-$, NO_3^-, Cl^-, Br^-, I^-, SO_4^{2-}, PO_4^{3-}, BO_3^{3-}, F^-, $C_2O_4^{2-}$

Paper 22-CHHP 616: Organic Chemistry -V

PRACTICAL   **Marks: 50**

1. Tests for following functional groups

2. Qualitative analysis of following types of unknown organic compounds

      1.   Carbohydrates
      2.   Primary, secondary and tertiary amines
      3.   Nitro compounds
      4.   Amides
      5.   Aryl halides
      6.   Hydrocarbons

Identification of the functional groups, C-C and C-N triple bonds, sp^3, sp^2 and sp hybridized C-H bonds by IR spectroscopy (IR spectra to be provided)

Paper 23-CHHP 617: Physical Chemistry -V

PRACTICAL **Marks: 50**

- Colourimetry
- Verification of Lambert-Beer's Law
- Determination of pK (indicator) for phenolphthalein or methyl red
- Study the formation of a complex between ferric and thiocyanate (or salicylate) ions.
- Study the kinetics of interaction of crystal violet with sodium hydroxide colourimetrically.
- Analysis of the given vibration-rotation spectrum of HCl(g)
- Record the UV spectrum of p-nitrophenol (in 1:4 ethanol:water mixture). Repeat after adding a small crystal of NaOH. Comment on the difference, if any.
- Record the U.V. spectrum of a given compound (acetone) in cyclohexane
  (a) Plot transmittance *versus* wavelength.

  (b) Plot absorbance *versus* wavelength.

  (c) Calculate the energy involved in the electronic transition in different units, i.e. cm^{-1}, kJ/mol, kcal/mol & eV.

Any other experiment carried out in the class.

Paper 24-CHHP 618: Application of Computers in Chemistry

PRACTICAL **Marks: 50**

Word processing:

Incorporating chemical structures into word processing documents, presentation graphics, on-line publication (www/html), multimedia animations, etc.

Handling numeric data: spreadsheet software (Excel), simple calculations, statistical analysis, plotting graphs using a spreadsheet (radial distribution curves for hydrogenic orbitals, gas kinetic theory, spectral data, pressure-volume curves of van der Waals gas, data from phase equilibria studies), graphical solution of equations, solving equations numerically (e.g. pH of a weak acid ignoring/ not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Numeric modelling, numerical curve fitting, linear regression (rate constants from concentration-time data, molar exinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric titrations), integration (e.g. entropy/enthalpy change from heat capacity data). Numerical solution of differential equations (e.g. kinetics).

Molecular modelling:

Visualization of 3D structures, calculation of molecular structures and properties (e.g., conformational energies of butane, rotation of 1,3-butadiene, distribution of isomers, energies of orbitals and total energy as a function of bond angle for H_2O, simulation of Diels-Alder reaction, S_N2 reactions).

Chemical information on the web. Chemical abstracts. Structures and properties.

Note: 1.Software: Microsoft Office, ChemOffice (Free alternatives: OpenOffice (www.openoffice.org), ISIS Draw (http://www.mdli.com; registration required), ArgusLab (www.planaria-software.com).

2. References: Internet, documentation of software.

These are representative projects. The students must be encouraged to explore other projects and prepare a presentation/poster based on their project. Internal assessment may be based on the project.