UNIVERSITY OF DELHI

DEPARTMENT OF CHEMISTRY

FOUR YEAR UNDERGRADUATE PROGRAMME

(Courses effective from Academic Year 2013-14)

SYLLABUS OF COURSES TO BE OFFERED

Discipline Courses I, Discipline Courses II

& Applied Courses

Note: The courses are uploaded as sent by the Department concerned. The scheme of marks will be determined by the University and will be corrected in the syllabus accordingly. Editing, typographical changes and formatting will be undertaken further.

Four Year Undergraduate Programme Secretariat
fouryearprog@gmail.com

CHEMISTRY
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DISCIPLINARY COURSE – I (DC-I)

The Disciplinary Course – I being offered in Chemistry for the Four Year Honours Programme would allow the student to gain in depth knowledge about the fundamental concepts and processes underlying the chemistry which forms the backbone of a number of chemical industries in the country. The course work shall train the students in the area of quantitative analysis of metal ions and other inorganic/organic compounds utilized in materials, polymers and food analysis. It would impart necessary skills in the area of extraction, separation, identification and synthesis of a variety of organic compounds utilized in chemical and pharma industry in India and abroad. Further it would familiarize the student in newer techniques of molecular modelling, electrochemical methods of analysis and use of IR, NMR and other spectroscopic techniques in the identification of inorganic and organic compounds at semi-micro level. It would bridge the physical and biological sciences.

DISCIPLINARY COURSE – II (DC-II)

The Disciplinary Course – II courses are for the students from other disciplines. The contents of DC-II courses are carefully designed to attract students from Physical Sciences as well as Biological Sciences.

APPLIED COURSE (AC)

The average life expectancy has increased over the years because of the positive ways in which chemistry has affected our lives. For example, the health care systems all over the world have improved considerably due to the new pharmaceutical drugs that are being synthesised and food and water being made safer for consumption etc. It will continue to play a leading role in order to provide a sustainable future to the increasing world population. Chemistry is one of the most exciting and fastest developing sciences and new knowledge in the field is being revealed every day. The curriculum of the four applied courses, namely, "Computer applications in chemistry", "Analytical Chemistry", "Pharmaceutical Chemistry" and "Green Chemistry" augment the strong knowledge chemistry provided in DC1. Graduates of this programme will have necessary skills to work in the industry or to pursue a higher degree of studies or a related field. These courses place a strong emphasis on hands on lab work which provides problem solving abilities required for successful career in pharmaceuticals, chemical industry, teaching, research, environmental monitoring, product quality, consumer goods industry, food products, cosmetics industry, etc. The importance of each of these four courses is further discussed in the syllabus.

CHEMISTRY: Detailed Syllabus

FIRST YEAR

SEMESTER-I

PAPER-1

THEORY

SECTION A – ORGANIC: BASIC CONCEPTS AND STEREOCHEMISTRY

Unit I: Basics of Organic Chemistry

Electron displacements- Inductive, electromeric, resonance, hyperconjugation.
Homolytic and heterolytic bond fission.
Reaction intermediate: Carbocations, carbanions, free radicals and carbenes- their shape and stability.
Electrophiles and nucleophiles.
Intermolecular forces of attraction: van der Waals forces, ion-dipole, dipole-dipole and hydrogen bonding.

Unit II: Stereochemistry

Isomerism in organic molecules- Structural and Stereoisomerism.
Molecular representations: Newman, Sawhorse, Wedge & Dash, Fischer projections and their interconversions.
Conformations and Conformational analysis: Ethane, n-butane, ethane derivatives, cyclohexane, monosubstituted and disubstituted cyclohexanes and their relative stabilities.
Geometrical isomerism in unsaturated and cyclic systems: cis–trans and, syn-anti isomerism, E/Z notations. Geometrical isomerism in dienes- Isolated and conjugated systems, determination of configurations.
Chirality and optical isomerism: Configurational isomers. Molecules with one or two chiral centres- constitutionally symmetrical and unsymmetrical molecules; Enantiomers and Diastereomers. Optical activity in absence of chiral centre – with illustrative examples (Allenes and Biphenyls). Meso compounds, racemic modifications and methods of their resolution; stereochemical nomenclature: erythro/threo, D/L and R/S nomenclature in acyclic systems. Measurement of optical activity: specific rotation.

Recommended Texts:

1. Morrison, Robert Thornton & Boyd, Robert Neilson *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
3. Finar, I. L. *Organic Chemistry* (*Volume 2: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education). Fifth Edition, 1975,
4. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*; First Edition, Wiley: London, 1994
5. Graham Solomons, T.W., Craig B. Fryhle *Organic Chemistry,* Ninth edition John Wiley & Sons, Inc. 2008.

SECTION B-PHYSICAL: GASES AND LIQUIDS

Unit I: Gaseous state

Kinetic molecular model of a gas: postulates; 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 molecular diameter from coefficient of viscosity of gases . Maxwell-Boltzmann distribution law (qualitative) 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); 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

Physical properties of liquids; surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Temperature variation of viscosity of liquids and comparison with that of gases.

Recommended texts:

1. Atkins, P.W. & Paula, J.D. *Physical Chemistry*, 9th Ed., Oxford University Press 2011.
2. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa 2004.
3. Mortimer, R. G. *Physical Chemistry 3rd Ed.*, Elsevier: NOIDA, UP 2009.
4. Barrow, G. M. *Physical Chemistry 5th Ed.*, Tata McGraw Hill: New Delhi 2006.
5. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall 2012.

6. Rogers, D. W. *Concise Physical Chemistry*, Wiley 2010.
7. Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. *Physical Chemistry 4th Ed.*, John Wiley & Sons, Inc. 2005.

PRACTICAL

SECTION A-ORGANIC: PURIFICATION OF ORGANIC COMPOUNDS & OPTICAL ACTIVITY

1. Purification of organic compounds by crystallization using the following solvents:
    a) Water
    b) Alcohol
    c) Alcohol-Water
2. Purity analysis by:
    a) Determination of the melting point (Kjeldahl method / electrically heated melting point apparatus).
    b) Determination of boiling point (distillation and capillary method).
3. To study the effect of non-volatile impurities on the melting point-mixed melting point of two unknown organic compounds.
4. Determination of optical activity by using polarimeter.

Recommended texts:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012)

SECTION B-PHYSICAL: MEASUREMENT OF SURFACE TENSION, VISCOSITY & AVOGADRO NUMBER

1. **Surface tension measurements.**
    a. Determination of surface tension of aqueous solutions by (i) drop number (ii) drop weight method.
    b. Study the variation of surface tension of detergent solutions with concentration.
2. **Viscosity measurement using Ostwald's viscometer**.
    a. Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
    b. To study the variation of viscosity of sucrose solution with concentration of solute.
3. **Determination of Avogadros number.**

Recommended Texts:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York 2003.
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York 2003.

PAPER – 2

INORGANIC: CHEMICAL BONDING I (ATOMIC STRUCTURE, PERIODICITY OF ELEMENTS, BASICS OF CHEMICAL BONDING), ACIDS AND BASES

THEORY

UNIT I: Atomic Structure

Wave mechanical model of hydrogen atom, de Broglie equation, Heisenberg's uncertainty principle and its significance, Schrödinger's wave equation (no derivation), significance of Ψ and Ψ^2. Quantum numbers and their significance. Radial wave functions. Sign of wave functions. Radial distribution curve and radial probability. Shapes of *s*, *p* & *d* orbitals. Pauli's exclusion principle, Hund's rule of maximum multiplicity, Aufbau principle and its limitations. Concept of extra stability of half and completely filled electronic configuration. Electronic configuration of elements.

UNIT II: Periodicity of Elements

Detailed discussion of the following properties of the elements, with reference to *s* & *p*- block elements.

i. Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.
ii. Atomic, covalent and ionic radial and their variation in groups and periods.
iii. Ionization enthalpy, factors affecting ionization enthalpy. Variation in groups and periods.
iv. Electron gain enthalpy, and its variation in groups and periods
v. Electronegativity, Pauling's and Mulliken-Jaffe's electronegativity scales, Variation of electronegativity with partial charge and hybridization

Unit III: Chemical Bonding-I

Ionic bond: General characteristics, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Lattice energy, Born-Lande equation with derivation. Madelung constant, Born-Haber cycle and its applications, Concept of solvation energy.

Unit IV: Acids and Bases

Bronsted- 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. Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
2. Douglas, B.E. & 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. & Selbin, J. *Theoretical Inorganic Chemistry*, ACS Publications 1962.
5. Huheey, J.E. *Inorganic Chemistry*, Prentice Hall 1993.
6. Manku, G.S. *Theoretical Inorganic Chemistry*, Tata McGraw hill, 1980.
7. Canham. *Descriptive Inorganic Chemistry 5th Ed*, W.H Freeman, 2010.
8. Shriver, D.D. & Atkins, P. *Inorganic Chemistry 3rd Ed.*, 1994.
9. Porterfield, H.W. *Inorganic Chemistry, 2nd Ed.*, Academic Press, 2005.

PRACTICAL

TITRIMETRIC ANALYSIS (VOLUMETRIC)

Acid-Base Titrations

Discussion of titration curves of different types of acid-base titrations. Choice of indicators.

i. Calibration of titrimetric apparatus.
ii. Estimation of NaOH (standard solution of oxalic acid to be prepared)
iii. Estimation of sodium carbonate (standard solution of sodium carbonate to be prepared)
iv. Estimation of carbonate and hydroxide present together in mixture.
v. Estimation of carbonate and bicarbonate present together in a mixture.
vi. Estimation of free alkali present in different soaps/detergents
vii. Estimation of total alkalinity in water samples from different sources.

Chromatography of Metal ions

Paper Chromatographic separation of following metal ions:

i. Ni (II) and Co (II)
ii. Fe (III) and Al (III)

Recommended texts:

1. Vogel, A.I., Fundamentals of Quantitative Analysis, 5th Ed., Addison Wesley longman., 1989.

SEMESTER - II

PAPER – 3

THEORY

SECTION A-ORGANIC: ALIPHATIC HYDROCARBONS

Unit I: Carbon-Carbon sigma bonds: Alkanes and Cycloalkanes

Alkanes: Preparation: Reduction reactions, Grignard reagent, coupling with organometallic compounds (Wurtz, Corey-House synthesis).
Physical properties: Melting point, boiling point, solubility and density.
Free radical substitution reactions: Halogenation, relative reactivity and selectivity. Allylic and benzylic bromination.
Cycloalkanes (C_3 to C_8): Relative stability, Baeyer strain theory and Sachse Mohr theory.

Unit II: Carbon-Carbon pi bonds: Alkenes, Alkynes and Alkadienes

Alkenes and Alkynes: Preparation: Elimination reactions- Mechanism of E_1, E_2, Saytzeff vs Hofmann eliminations.
Physical properties: Melting point, boiling point, solubility and density.
Electrophilic addition to alkenes and alkynes: Addition of hydrogen halides, halogens, water, hypohalous acid (Markovnikov's rule and peroxide effect).
Mechanism of hydroboration-oxidation and oxymercuration-demercuration.
Oxidative cleavage of alkenes and alkynes.
Stereochemical aspects of organic reactions: Chemical and catalytic hydrogenation of alkenes, hydroxylation, carbene addition, halogen and halogen acid addition, dehydrohalogenation.
Acidity of alkynes and their associated reactions as nucleophiles.
Relative reactivities of alkenes and alkynes towards electrophilic addition reactions.
Alkadienes: 1,2- and 1,4- addition reactions in conjugated dienes, Diels-Alder reaction (excluding stereochemical aspects).

Recommended Texts:

1. Morrison, Robert Thornton & Boyd, Robert Neilson *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
3. Finar, I. L. *Organic Chemistry* (*Volume 2: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education). Fifth Edition, 1975,
4. Graham Solomons, T.W., Craig B. Fryhle *Organic Chemistry*, Ninth edition John Wiley & Sons, Inc. 2008.

SECTION B-INORGANIC: CHEMICAL BONDING-II

i. Covalent bond: Valence Bond theory (Heitler-London and Pauling approach). Concept of hybridization, Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule. 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, bond energies.

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

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

iv. Molecular orbital theory: Molecular orbital diagrams of homo$^-$ and hetero nuclear diatomic molecules N_2, O_2, C_2, B_2, F_2, CO, NO, and their ions; HCl, (idea of s-p mixing to be given).

v. Metallic bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators.

vi. 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 (inter and intra) and its application (melting, boiling points and solubility).

Recommended Texts:

1. Huheey, J.E. *Inorganic Chemistry*, Prentice Hall 1993.
2. Douglas, B.E. & McDaniel, 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. Porterfield, H.W. *Inorganic Chemistry*, Second Edition, Academic Press, 2005.

PRACTICAL

SECTION A- ORGANIC: PREPARATION OF ORGANIC COMPOUNDS AND CHROMATOGRAPHY

1. Chromatography, technique for separation and purity analysis of organic compounds.
   i. Separation of a mixture of two amino acids by ascending and radial paper chromatography.
   ii. Separation of a mixture of two carbohydrates by ascending and radial paper chromatography.

iii. Separation of a mixture of *o*- and *p*-nitrophenol or *o*- and *p*-aminophenol by thin layer chromatography (TLC).

2. Diels Alder reaction:
   i. of anthracene and maleic anhydride.
   ii. of furan and maleic acid.

3. Bromination of trans stilbene.

Recommended Texts:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education 2009.
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson 2012.

SECTION B- INORGANIC: OXIDATION – REDUCTION TITRIMETRY

Oxidation- Reduction Titrimetry:

Concept of electrode potential, Redox indicators like diphenylamine and N-phenyl anthranilic acid.

i. Estimation of Fe(II) using standardized $KMnO_4$ solution (standard solution of Mohr's salt to be prepared).
ii. Estimation of oxalic acid and sodium oxalate in a given mixture. (standard solution of oxalic acid to be prepared)
iii. Estimation of Fe (II) with $K_2Cr_2O_7$ using diphenylamine as internal indicator (standard solution of Mohr's salt to be prepared).
iv. Estimation of Potassium dichromate with Mohr's salt using N-phenyl anthranilic acid as internal indicator (standard solution of Potassium dichromate to be prepared).
v. Estimation of iron content in drug / ore / alloy using potassium dichromate.

Recommended Text:

1. Vogel, A.I., Fundamentals of Quantitative Analysis, 5th Ed., Addison Wesley longman., 1989.

PAPER-4

PHYSICAL: CHEMICAL THERMODYNAMICS & SYSTEMS OF VARIABLE COMPOSITION

THEORY

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 of gases, liquids and solids; 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.

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

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

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.

Recommended texts:

1. Peter, A. & Paula, J. de. *Physical Chemistry 9th Ed.*, Oxford University Press 2011.
2. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa 2004.
3. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall 2012.
4. McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi 2004.
5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics.* CRC Press: NY 2011.

6. Levine, I .N. *Physical Chemistry 6th Ed.,*Tata Mc Graw Hill 2010.
7. Metz, C.R. *2000 solved problems in chemistry,* Schaum Series 2006.

PRACTICAL

PHYSICAL: 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 the enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
c. Determination of the enthalpy of ionization of ethanoic acid.
d. Determination of integral enthalpy (endothermic and exothermic) of 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.

Recommended Texts:

1. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi 2011.
2. Athawale, V. D. & Mathur, P. *Experimental Physical Chemistry* New Age International: New Delhi 2001.

SECOND YEAR

SEMESTER-III

PAPER-5

THEORY

SECTION A-INORGANIC: PRINCIPLES OF METALLURGY and CHEMISTRY OF s-BLOCK ELEMENTS

Unit I: General principles of metallurgy

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy. Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining.

Unit II: Chemistry of s-block elements:

i. General Characteristics: Density, melting point, flame color, reducing nature, diagonal relationships and anomalous behaviour of first member of each group.
ii. Oxidation states with reference to elements in unusual and rare oxidation states (alkali metal anions)
Reactions of alkali and alkaline earth metals with oxygen, hydrogen, nitrogen and water.
iii. Common features such as ease of formation, thermal stability, solubility and % ionic character of thse following Alkali Metal and Alkaline Earth Metal Compounds
Hydrides, Oxides, peroxides, superoxides, Carbonates, Bicarbonates, Nitrates, Sulphates.
iv. Complex Formation tendency of *s*-block elements , Structure of the following complexes
Crown ethers, cryptates, basic beryllium acetate, beryllium nitrate, salicyaldehyde/acetylacetonato complexes of Group I, EDTA complexes of calcium and magnesium.
v. Solution of alkali metals in liquid ammonia and their properties.
vi. Uses of alkali metals with special reference to lithium in drugs & batteries.

Recommended Texts:

1. Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
2. Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of Inorganic Chemistry 3rd Ed.*, John Wiley Sons, N.Y. 1994.

3. Greenwood, N.N. & Earnshaw. *Chemistry of the Elements*, Butterworth-Heinemann. 1997.
4. Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.
5. Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry 4th Ed.,* Pearson, 2010.
6. Shriver & Atkins, *Inorganic Chemistry 5th Ed.*

SECTION B-PHYSICAL: CHEMICAL and IONIC EQUILIBRIA

Unit I: Chemical equilibrium

Criteria of thermodynamic equilibrium, chemical equilibria in ideal gases. Thermodynamic derivation of relation between Gibbs energy of reaction and reaction quotient. Equilibrium constants, relations between the various equilibrium constants K_p, K_c and K_x, and their quantitative dependence on temperature, pressure and concentration. Gibbs energy of mixing and spontaneity. Le Chatelier principle (quantitative treatment).

Unit II: 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 triprotic acids (exact treatment of monoprotic acid). Salt hydrolysis- calculation of hydrolysis constant, degree of hydrolysis and pH for different salts.
Buffer solutions: derivation of Henderson–Hesselbelch equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry.
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 in case of strong acid and strong base). Theory of acid–base indicators; selection of indicators and their limitations.

Recommended texts:

1. Peter Atkins & Julio De Paula, *Physical Chemistry 9th Ed.,* Oxford University Press 2010.
2. Castellan, G. W. *Physical Chemistry*, 4th Ed., Narosa 2004.
3. McQuarrie, D. A. & Simon, J. D., *Molecular Thermodynamics*, Viva Books Pvt. Ltd.: New Delhi 2004.
4. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.,* Prentice-Hall 2012.
5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics.* CRC Press: NY 2011.
6. Zundhal, S.S. *Chemistry concept and applications* Cengage India 2011.

PRACTICAL

SECTION A-INORGANIC: IODO AND IODIMETRIC TITRATIONS

i. Estimation of Cu (II) using sodium thiosulphate solution (Iodometrically).
ii. Estimation of $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodometrically).
iii. Estimation of antimony in tartar-emetic iodimetrically
iv. Estimation of available chlorine in bleaching powder iodometrically.
v. Estimation of dissolved oxygen in water samples.

Recommended text:

1. Vogel, A.I., Fundamentals of Quantitative Analysis, 5^{th} Ed., Addison Wesley longman., 1989.

SECTION B-PHYSICAL: pH METRY

a) Study the effect of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
b) Preparation of buffer solutions of different pH
    i. Sodium acetate-acetic acid
    ii. Ammonium chloride-ammonium hydroxide
c) pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.
d) Determination of dissociation constant of a weak acid.

Recommended Texts:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8^{th} Ed.*; McGraw-Hill: New York 2003.
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3^{rd} Ed.;* W.H. Freeman & Co.: New York 2003.

PAPER – 6

ORGANIC: AROMATIC HYDROCARBONS, HALOGENATED HYDROCARBONS, ALCOHOLS AND PHENOLS

THEORY

Unit I: Aromatic Hydrocarbons

Benzene: Kekule structure, stability of benzene, resonance energy.
Aromaticity: Hückel's rule, aromaticity in benzene and other cyclic systems with examples of aromatic, non-aromatic and antiaromatic systems of cyclic hydrocarbons (C_3 to C_8) excluding heterocyclic compounds.
Properties of benzene: Electrophilic substitution reactions: halogenation, nitration, sulphonation, Friedel–Crafts alkylation and its limitations, Friedel Crafts acylation.
Addition reactions: Addition of chlorine and hydrogen.
Oxidation reactions: With oxygen and ozone, mercuration and Birch reduction.
Effect of sustituents on electrophilic substitution reactions, orientation and reactivity in monosubstituted and disubstituted benzene.
Oxidation and halogenation (ring vs side chain) of alkylbenzenes.
Toxicity of benzene vs toluene.

Unit II: Chemistry of Halogenated Hydrocarbons

Alkyl halides: Preparation, physical properties, nucleophilic substitution reactions – S_N1, S_N2 and S_Ni mechanism with stereochemical aspects, factors affecting nucleophilic substitution, elimination vs substitution, nucleophilicity vs basicity.
Aryl halides: Preparation, physical properties and nucleophilic aromatic substitution: S_NAr, elimination-addition mechanism.
Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.
Organometallic compounds of Mg and Li: synthetic uses.

Unit III: Alcohols, Phenols, Ethers and Epoxides

Alcohols: Preparation, relative reactivity of primary, secondary and tertiary alcohols. Alcohols as acids and bases.
Reactions of alcohols: With hydrogen halides, phosphorous halides, thionyl chloride and ammonia.
Oxidation of alcohols: Dehydrogenation and dehydration, Lucas reagent test, Victor Meyer test and Iodoform test.
Glycols: Preparation and reactions: Oxidation, Pinacol–Pinacolone rearrangement.
Phenols: Preparation and reactions: Acidity and factors affecting acidity of phenols.
Acylation of phenol, ring substitution reactions,Riemer–Tiemann reaction, Kolbe reaction, Fries and Claisen rearrangements.

Ethers and Epoxides: Preparation and reactions with acid. Acid and base catalysed ring opening of epoxides.

Recommended Texts:

1. Morrison, Robert Thornton & Boyd, Robert Neilson *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
3. Graham Solomons, T.W., Craig B. Fryhle *Organic Chemistry*, Seventh edition John Wiley & Sons, Inc. 2000.

PRACTICAL

ORGANIC: FUNCTIONAL GROUP DETECTION AND ORGANIC PREPARATION

1. Functional group tests for alcohols and phenols.
2. Organic preparations:
   i. 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) by any one method:
      a. Using conventional method.
      b. Using green approach
   ii. Benzolyation of one of the following amines (aniline, *o*-,*m*-,*p*- toluidines and *o*-,*m*-,*p*- anisidine) and one of the following phenols (β-naphthol, resorcinol, p-cresol) by Schotten-Baumann reaction.
   iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
   iv. Bromination of any one of the following:
      a. Acetanilide by conventional methods
      b. Acetanilide using green approach (Bromate-bromide method)
   v. Nitration of any one of the following:
      a. Acetanilide/nitrobenzene by conventional method
      b. Salicylic acid by green approach (using ceric ammonium nitrate).
   vi. Selective reduction of meta dinitrobenzene to m-nitroaniline.
   vii. Reduction of p-nitrobenzaldehyde by sodium borohydride.

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 and TLC.

Recommended Texts:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education 2009.
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, *5th Ed.*, Pearson 2012.
3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press 2000.
4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press 2000.

SEMESTER – IV

PAPER-7

THEORY

SECTION A-ORGANIC: CARBONYL COMPOUNDS AND CARBOXYLIC ACIDS

Unit I: Carbonyl Compounds

Aldehydes and Ketones: Preparations, physical properties and reactions.
Nucleophilic addition: Mechanism and relative reactivity of aldehydes and ketones. Test for aldehydes & ketones.
Nucleophilic addition- elimination: reaction with ammonia derivatives.
Mechanisms of Aldol, Claisen Schmidt, Benzoin and Perkin condensations, Cannizzaro, Wittig, Knoevenegel and Reformatsky reactions, Beckmann and Benzil-Benzilic acid rearrangements.
Oxidation (including Baeyer Villiger oxidation) and Reduction.
α,β-Unsaturated Carbonyl Compounds: Electrophilic and nucleophilic addition reactions including Michael addition.

Unit II: Carboxylic Acids and their Derivatives

Monocarboxylic acids: Preparation, physical properties and reactions. Conversion into fuctional derivatives, Hell-Volhard-Zelinsky reaction.
Acidity of carboxylic acids, effect of substitution on acid strength of aliphatic and aromatic acids, ortho effect.
Acid chlorides, Anhydrides, Esters and Amides: Preparation and reactions, ester hydrolysis, transesterification, Claisen, Dieckmann, and Darzens Glycedic ester condensations.
Relative reactivities of acid derivatives towards nucleophiles.
Dicarboxylic acids, Unsaturated acids (maleic and fumaric acid) **and Hydroxy acids**: Typical reactions and uses.

Recommended Texts:

1. Morrison, Robert Thornton & Boyd, Robert Neilson *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
3. Graham Solomons, T.W., Craig B. Fryhle *Organic Chemistry*, Ninth edition John Wiley & Sons, Inc. 2008.

SECTION B- PHYSICAL: CHEMICAL KINETICS & CATALYSIS

Unit I: Chemical Kinetics

Order and molecularity of a reaction. Differential and integrated form of rate expressions up to second order reactions. Experimental methods of the determination of order of a reaction, 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, Lindemann mechanism. Collision theory of reaction rates, qualitative treatment of the theory of absolute reaction rates.

Unit II: Catalysis

Types of catalysts, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis.

Recommended Texts:

1. Atkins, P. W. & Paula, J. de Atkins *Physical Chemistry 9th Ed.,* Oxford University Press 2011.
2. Ball, D. W. *Physical Chemistry, 3rd Ed.*, Cengage India.2012.
3. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa 2004.
4. Laidler, K. J. *Chemical Kinetics*, Pearson Education: New Delhi 2004.
5. Rogers, D. W. *Concise Physical Chemistry* Wiley 2010.
6. Thomas, E. & Philip, R. *Thermodynamics: Statistical Thermodynamics and Kinetics, 1st Ed.,* Pearson Education 2007.
7. Zumdahl, S.S. Chemistry concepts and applications Cengaga India 2011.

PRACTICAL

SECTION A-ORGANIC: FUNCTION GROUPS DETECTION AND ORGANIC PREPARATION

1. Functional group test for carbonyl group and carboxylic acid group.
2. Organic preparations:
   i. Hydrolysis of amides and esters.
   ii. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
   iii. *S*-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
   iv. Aldol condensation using either conventional or green method.
   v. Benzil-Benzilic acid rearrangement.

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 and TLC.

Recommended Texts:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.,* Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis,* University Press (2000).
4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis,* University Press (2000).

SECTION B- PHYSICAL: KINETICS OF SELECTED REACTIONS

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.
   b. Saponification of ethyl acetate.
   c. Iodide-persulphate reaction.
3. Compare the strengths of HCl and H_2SO_4 by kinetics of hydrolysis of methyl acetate.

Recommended Texts:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York 2003.
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York 2003.
4. Sindhu,P.S. *Practicals in Physical Chemistry 1st Ed.* Macmillan: India 2006.

PAPER-8

INORGANIC: CHEMISTRY OF p-BLOCK ELEMENTS.

THEORY

Unit I: Chemistry of p-block elements

Electronic configuration, atomic and ionic size, metallic/non metallic character, melting point, ionization enthalpy, electron gain enthalpy, electronegativity. Allotropy, inert pair effect, diagonal relationship between Boron and Silicon and anomalous behaviour of first member of each group.

Unit II: Structure, bonding and properties: acidic/basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, action of heat

Hydrides: Hydrides of group 13 (only Diborane), group 14, group 15 (EH_3 where E=N, P, As, Sb, Bi), group 16 and group 17.

- Oxides: Oxides of nitrogen, phosphorus, sulphur and chlorine.
- Oxoacids: Oxoacids of nitrogen, phosphorus, peroxoacids of sulphur, chlorine.
- Halides: Halides of carbon, silicon, nitrogen and phosphorus.

Preparation, property, structure and uses of the following compounds

- Boric acid, borates, boron nitrides, borazine.
- Silicates, Ceramic materials, silicones, graphitic compounds, intercalation compounds of graphite.
- Phosphonitrilic halides $\{(PNCl_2)_n$ where n = 3 and 4$\}$
- Interhalogen and pseudohalogen compounds.
- Clatharate compounds of noble gases, Xenon fluorides (M.O. treatment of XeF_2).

Recommended Texts:

1. Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
2. Douglas, B.E. & Mc Daniel, D.H. *Concepts & Models of Inorganic Chemistry*, Oxford, 1970
3. Greenwood, N.N. & Earnshaw, *Chemistry of the Elements*, Butterworth-Heinemann. 1997.
4. Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.
5. Gary L. Miessler, Donald A. Tarr, *Inorganic Chemistry, 4th Ed.*, Pearson, 2010.

PRACTICAL

INORGANIC: COMPLEXOMETRIC TITRATIONS

i. Complexometric estimation of Mg^{2+} using EDTA.
ii. Complexometric estimation of Zn^{2+} using EDTA.
iii. Estimation of total, temporary and permanent hardnesss of water samples.
iv. Estimation of Ca^{2+} in solution by (substitution method) using Erio-chrome black-T as indicator.
v. Estimation of Ca^{2+} /Mg^{2+} in drugs/ milk/ biological samples by Back titration.
vi. Complexometric estimation of Zn^{2+} using Xylenol orange as indicator.
vii. Complexometric estimation of Al^{3+} using Erio-chrome black-T as indicator.
viii. Complexometric estimation of mixture of Zn^{2+} and Mg^{2+} in a sample solution using Xylenol orange and Eriochrome black-T as indicator
ix. Complexometric estimation of mixture of Al^{3+} and Mg^{2+} in a sample solution using masking agent.
x. Estimation of $BaSO_4$ by EDTA back titration using Eriochrome black-T as indicator.

Recommended text:

1. Vogel, A.I., Fundamentals of Quantitative Analysis, 5^{th} Ed., Addison Wesley longman., 1989.

THIRD YEAR

SEMESTER - V

PAPER – 9

INORGANIC: d-BLOCK ELEMENTS, COORDINATION CHEMISTRY, LANTHANIDES & ACTINIDES

THEORY

Unit I: Transition elements

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, and ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer diagrams). Comparison of 3d elements with 4d & 5d elements.

Various oxidation states, their oxidizing and reducing nature and stability w.r.t. Ti, V, Cr, Mn, Fe and Co. Structure and chemical reactivity of following compounds: chromate, dichromate and chromium trioxide, $KMnO_4$, peroxo compounds of chromium, V_2O_5, $K_4[Fe(CN)_6]$, $K_3[Fe(CN)_6]$, $Na_3[Co(NO_3)_6]$, $Na_3[Fe(CN)_5NO]$

Unit II: Coordination chemistry

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. 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, concept of pairing energies and lattice energy, color and magnetic properties , factors affecting the magnitude of 10 Dq (Δo, Δt). Octahedral vs. Tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Elementary idea of Ligand field and MO Theory.

Unit III: Lanthanides and actinides

Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction. Separation of lanthanoides (ion-exchange method only).

Recommended Texts:

1. Purecell, K.F. & Kotz, J.C. *Inorganic Chemistry*, W.B. Saunders Co. 1977.
2. Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann,1997.
3. Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
4. Gary L. Miessler, Donald A. Tarr, *Inorganic Chemistry, 4/E,* Pearson, 2010.
5. Huheey, J.E. *Inorganic Chemistry*, Prentice Hall 1993

PRACTICAL

INORGANIC: GRAVIMETRIC ANALYSIS AND INORGANIC PREPARATION

Gravimetric Analysis:

i. Estimation of nickel (II) using Dimethylglyoxime (DMG).
ii. Estimation of copper as CuSCN
iii. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.

Inorganic Preparations:

i. Tetraamminecopper (II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$
ii. *Cis* and *trans* $K[Cr(C_2O_4)_2.(H_2O)_2]$ Potassium dioxalatodiaquachromate (III)
iii. Tetraamminecarbonatocobalt (III) ion
iv. Potassium tris(oxalate)ferrate(III)

Spectophotometric estimation:

i. To draw calibration curve (absorbance at λ_{max} vs. Concentration) for various concentrations of a given coloured compound and to estimate the concentration of the same in a given solution.
ii. Spectrophotometric estimation of Ferrous ion by using 1,10-phenanthroline
iii. Determination of composition of Fe (III)-salicyclic acid complex by Job's method.

Recommended Text:

1. Vogel, A.I., Fundamentals of Quantitative Analysis, 5th Ed., Addison Wesley longman., 1989.

PAPER-10

ORGANIC: COMPOUNDS, CONTAINING ACTIVE METHYLENE, NITROGEN CONTAINING FUNCTIONAL GROUPS; POLYNUCLEAR HYDROCARBONS AND HETEROCYCLES

THEORY

Unit I: Active methylene compounds

Concept of Keto-enol tautomerism, preparation, reactions and synthetic applications of diethyl malonate and Ethyl acetoacetate: Synthesis of carboxylic acids, dicarboxylic acids, β-keto acids, diketones and heterocyclic compounds.

Unit II: Compounds with Nitrogen Containing Functional Groups

Nitro compounds: Preparation, physical properties and reactions.
Alkyl nitriles and Isonitriles: Preparation, physical properties and reactions.
Aliphatic and aromatic amines: Preparation: rearrangement reactions (Lossen, Curtius,Schmidt and Hofmann bromamide), Gabriel phthalimide synthesis, reduction (including reductive amination).
Structure, physical properties and basic character of amines: Effects of solvent, substituents and steric inhibition of resonance.
Reactions**:** Reactions involving nucleophilic character:Alkylation, acylation, Mustard oil reaction, Carbylamine reaction, Mannich reaction, Eschwieler Clark methylation, Hofmann exhaustive methylation, Hofmann elimination (stereochemistry and comparison with Cope reaction)**,** oxidation reactions, coupling reactions and electrophilic substitution in aromatic Amines.
Separation of 1^{o}, $2^{o}$and 3^{o} amines (Hofmann method and Hinsberg method).
Diazonium salts: Preparation and their applications.

Unit III: Polynuclear Hydrocarbons

Introduction to polynuclear hydrocarbons**.**
Structure elucidation of Naphthalene.
Preparation and reactions of Naphthalene, Anthracene and Phenanthrene.

Unit IV: Heterocyclic Compounds

Heterocyclic compounds: Classification, nomenclature and their importance in medicine and agrochemicals.
Structure, basic character and aromaticity in 5- and 6-membered rings containing one heteroatom and condensed heterocyclics. Comparative study of basicity of heterocyclic compounds.

Synthesis and reactions of one heteroatom containing five membered ring and its benzofused ring: Furan, Pyrrole (Paal-Knorr synthesis, Knorr Pyrrole synthesis, Hantzsch synthesis), Thiophene, Indole(Fischer indole synthesis and Madelung synthesis)

Synthesis and reaction of one hetero atom containing six membered ring and its benzofused ring: Pyridine (Hantzsch synthesis), Quinoline and Isoquinoline (Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction).

Recommended Texts:

1. Morrison, Robert Thornton & Boyd, Robert Neilson *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
3. Finar, I. L. *Organic Chemistry* (*Volume 2: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education) Fifth Edition , 1975.
4. Graham Solomons, T.W., Craig B. Fryhle *Organic Chemistry*, Ninth edition John Wiley & Sons, Inc. 2008.
5. Acheson, R.M. *Introduction to the Chemistry of Heterocyclic compounds*, John Welly & Sons ,Third Edition 1976 .

PRACTICAL

ORGANIC: FUNCTIONAL GROUP ANALYSIS AND QUALITATIVE ANALYSIS

1. Detection of extra elements.
2. Functional group test for nitro, amine and amide groups.
3. Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols and carbonyl compounds)

Recommended Texts:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education 2009.
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson 2012/
3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press 2000.
4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press 2000.

PAPER-11

PHYSICAL: ELECTROCHEMISTRY

THEORY

Unit I: Electrolytic Conductance

Electrolytic and metallic conductance. 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.

Ionic velocities, mobilities and their determinations. Grotthus conductance, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Anomalous transference numbers. Waldens rule.

Application of EMF measurements in determining (i) Gibbs energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinhydrone and glass electrodes.

Unit II: Chemical Cells

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 types of half-cells. Determination of exact value of half-cell potential, dissociation constant of weak acid, ionic product of water by graphical method.

Application of EMF measurements in determining (i) Gibbs energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone and glass electrodes.

Concentration cells with and without transference, liquid junction potential; Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation).

Recommended texts:

1. Atkins, P.W & Paula, J.D. *Physical Chemistry*, 9th Ed., Oxford University Press 2011.
2. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa 2004.
3. Mortimer, R. G. *Physical Chemistry 3rd Ed.*, Elsevier: NOIDA, UP 2009.
4. Barrow, G. M., *Physical Chemistry 5th Ed.*, Tata McGraw Hill: New Delhi 2006.
5. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall 2012.
6. Rogers, D. W. *Concise Physical Chemistry* Wiley 2010
7. Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. *Physical Chemistry 4th Ed.*, John Wiley & Sons, Inc. 2005.

PRACTICAL

PHYSICAL: CONDUCTOMETRY AND POTENTIOMETRY

Conductometry

1. Determination of cell constant
2. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
3. To perform the following conductometric titrations:
    i. Strong acid vs. strong base
    ii. Weak acid vs. strong base
    iii. Mixture of strong acid and weak acid vs. strong base
    iv. Strong acid vs. weak base

Potentiometry

II To perform the following potentiometric titrations:
    i. Strong acid vs. strong base
    ii. Weak acid vs. strong base
    iii. Dibasic acid vs. strong base
    iv. Potassium dichromate vs. Mohr's salt

Recommended Texts:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York 2003.
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York 2003.

SEMESTER-VI

PAPER-12

INORGANIC: ORGANOMETALLIC, BIO-INORGANIC CHEMISTRY

THEORY

Unit I: Theoretical Principles in Inorganic Qualitative Analysis (H_2S Scheme)

Basic principles involved in analysis of cations and anions and solubility products, common ion effect. Principles involved in separation of cations into groups and choice of group reagents. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after Group II.

Unit II: Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands.

Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

Unit III: Bioinorganic Chemistry

Metal ions present in the biological system and classification on the basis of action (essential, non-essential, trace, toxic). Classification of metallobiomolecules (enzymes, transport and storage proteins and non proteins). Na – K pump, a brief idea of ionophores. Importance of Zn as a biocatalyst. Metalloenzymes involving Zn – carbonic anhydrase, and carboxypeptidase A. Structure of the active site and function of these enzymes in brief.

Importance of iron in the human system with reference to haemoglobin and myoglobin. Role of haemoglobin as an oxygen carrier, Perutz Mechanism for oxygenation of haemoglobin,

Cooperative Effect, Bohr Effect, comparison of oxygen saturation curves of haemoglobin and myoglobin. Storage and transport of iron in humans – Ferritin and Transferrin.
Chelating agents in medicine: Use of chelating agents like EDTA, BAL and D- penicillamine in metal poisoning. Anticancer activity of Cisplatin.

Recommended Texts:

1. Vogel, A.I. *Qualitative Inorganic Analysis*, Longman, 1972
2. Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall, 1996-03-07.
3. Cotton, F.A. G.; Wilkinson & Gaus, P.L. *Basic Inorganic Chemistry 3rd Ed.;* Wiley India,
4. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed.*, Harper Collins 1993, Pearson,2006.
5. Sharpe, A.G. *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005
6. Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry3rd Ed.*, John Wiley and Sons, NY, 1994.
7. Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements*, *Elsevier 2nd Ed*, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
8. Lee, J.D. *Concise Inorganic Chemistry 5th Ed.*, John Wiley and sons 2008.
9. Powell, P. *Principles of Organometallic Chemistry*, Chapman and Hall, 1988.
10. Shriver, D.D. & P. Atkins, *Inorganic Chemistry 2nd Ed.*, Oxford University Press, 1994.
11. Bertini, I.; Gray, H.B.; Lippard, S.J. & Valentine, J.S. *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., 1998.
12. Lippard, S.J. & Berg, J.M. *Principles of Bioinorganic Chemistry*, Panima Publishing Corporation, 1997.
13. Hughes, M.N. *Inorganic Chemistry of Biological Processes*, John Wiley and Sons, London, 1981.

PRACTICAL

INORGANIC: QUALITATIVE SEMIMICRO ANALYSIS

Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:
CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-},$S_2O_3^{2-}$, CH_3COO^-, F^-,Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, $Al^{3+,}$, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+},Sr^{2+}, Ca^{2+}, Mg^{2+}
Mixtures should preferably contain one interfering anion, **or** insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) **or** combination of anions e.g. $CO_3^{2-}$and SO_3^{2-}, $NO_2^-$and NO_3^-, Cl^- and Br^-, Cl^- and I^-, $Br^-$and I^-, NO_3^- and Br^-, NO_3^- and I^-.
Spot tests should be done whenever possible.

Recommended Text:

1. Svehla, Vogel, A.I. *Qualitative Inorganic Analysis*, Longman, 1972
2. G. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall, 1996-03-07.

PAPER – 13

ORGANIC: CARBOHYDRATES, SPECTROSCOPY AND DYES

THEORY

Unit I: Carbohydrates

Occurrence, classification, reducing and non reducing sugars, reactions and their biological importance.

Monosaccharides: Structure elucidation, relative and absolute configuration of glucose and fructose, co-relation of configuration, characteristic reactions of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures and conformational analysis (elementary idea, anomeric effect), configuration on C-1 in glucose, interconversions of aldoses and ketoses, Kiliani-Fischer synthesis, Ruff's degradation and Wohl's method.

Disaccharides: Nomenclature, applications and structural distinction of maltose, lactose and sucrose; Invert sugar.

Polysaccharides: Elementary treatment of starch, cellulose and glycogen (comparative study of their structures) and their application.

Unit II: Spectroscopy

Introduction to spectroscopy: Electromagnetic radiation, fundamental definitions, electromagnetic spectrum, introduction to concepts of absorption and emission spectroscopy, Beer-Lambert law.

UV spectroscopy: Types of electronic transitions, UV spectrum, λ_{max}, ϵ_{max}, chromophores, auxochromes, bathochromic shift, hypsochromic shift (definitions and elementary examples) and solvent effect. Characteristic UV transitions in common functional groups.

General applications of UV spectroscopy including distinction between cis-trans isomers.

Woodward rules for calculating λ_{max} in following systems:

- Conjugated dienes: alicyclic, homoannular, heteroannular.
- α,β-Unsaturated aldehydes and ketones.
- Extended conjugated systems: dienes, aldehydes and ketones.

IR Spectroscopy: Fundamental and non-fundamental molecular vibrations, IR spectrum, fingerprint and group frequency regions and their significance, Hooke's law and vibrational frequency. Factors affecting vibrational frequency in organic compounds.

Characterization of functional groups: alkanes, alkenes, alkynes (only alicyclic systems), aldehydes, ketones, carboxylic acids and their derivatives, hydroxy compounds and amines. Study of hydrogen bonding.

PMR spectroscopy: Basic principles of NMR spectroscopy, PMR scale, chemical shifts (concept of shielding and deshielding), factors influencing chemical shifts, simple spin-spin

couplings, coupling constant, chemical shift equivalence, anisotropic effects in alkenes, alkynes, aldehydes and aromatics. Interpretation of PMR spectra of simple compounds.

Application of UV, IR and PMR in solving structures of simple organic molecules.

Unit III: Dyes

Colour and constitution of dyes**:** Witt's theory, quinonoid theory, valence bond theory (VBT) and molecular orbital theory (MOT).
Classification of dyes with examples on the basis of mode of application**:** Acidic, basic, direct, mordant, vat developed and dispersed dyes.
Classification of dyes with examples on the basis of structure**:** Azo dyes, triphenyl methane dyes, phthalein dyes, xanthene dyes and natural dyes.
Synthesis and uses of following dyes:
Methyl orange, malachite green, phenolphthalein.
Structure elucidation and synthesis of alizarin and indigo.

Recommended Texts:

1. Morrison, Robert Thornton & Boyd, Robert Neilson *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
3. Finar, I. L. *Organic Chemistry* (*Volume 2: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Fifth Edition, 1975.
4. Graham Solomons, T.W., Craig B. Fryhle *Organic Chemistry*, Ninth edition John Wiley & Sons, Inc. 2008.
5. Kemp, W. *Organic Spectroscopy*, Palgrave Macmillan Education Ltd, Second Edition, 1987.

PRACTICAL

ORGANIC: QUALITATIVE ANALYSIS, PREPARATION AND USE OF IR AND NMR

1. Analysis of Carbohydrate: aldoses and ketoses, reducing and non-reducing sugars.
2. Qualitative analysis of unknown organic compounds containing monofunctional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, for e.g. salicylic acid, cinnamic acid, nitrophenols etc.
3. Identification of simple organic compounds by IR spectroscopy and PMR spectroscopy (Spectra to be provided).
4. Preparation of methyl orange.

Recommended Texts:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education 2009.
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, *5th Ed.*, Pearson 2012.

3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press 2000.
4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press 2000.

PAPER-14

PHYSICAL: PHASE EQUILIBRIA & BINARY SOLUTIONS

THEORY

Unit I: Phase equilibria

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

Phase diagrams for two component systems involving eutectic, congruent and incongruent melting points and solid solutions.

Three component system: water-chloroform-acetic acid system only.

Unit: II: 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, immiscible pairs, steam distillation. Nernst distribution law: its derivation and applications.

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, 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. Glasses and liquid crystals.

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* Cengage India 2012.
3. Castellan, G. W. *Physical Chemistry 4th Ed.,* Narosa 2004.
4. Mortimer, R. G. *Physical Chemistry 3rd Ed.,* Elsevier: NOIDA, UP 2009.
5. Levine, I. N. *Physical Chemistry 6th Ed.,* Tata McGraw-Hill 2011.
6. Metz, C. R. *Physical Chemistry 2nd Ed.,* Tata McGraw-Hill 2009.

PRACTICAL

PHYSICAL: DETERMINATION OF CRITICAL SOLUTION AND PHASE EQUILIBRIA

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

II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method:
    a. simple eutectic and
    b. congruently melting systems.

III. Indexing of a given powder diffraction pattern of a cubic crystalline system.

IV. Distribution of acetic/ benzoic acid between water and cyclohexane.

Recommended Texts:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York 2003.
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York 2003.
4. Sindhu,P.S. *Practicals in Physical Chemistry 1st Ed.* Macmillan: India 2006.

FOURTH YEAR

SEMESTER-VII

PAPER-15

THEORY

SECTION A-INORGANIC: REACTION RATES & MECHANISM

Unit 1: Reaction Kinetics and Mechanism:

Introduction to Inorganic Reaction Mechanism. Substitution reactions in square planar complexes, Trans- effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes.

Unit II: Introduction to catalysis of chemical reactions by organometallic compounds

Discuss the processes that commonly feature in the mechanism of following reactions:

1. Alkene hydrogenation (Wilkinsons Catalyst)
2. Hydroformylation (Co salts)
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Synthesis gas by metal carbonyl complexes

Reference text:

1. Huheey, J. E.; Keiter, E. A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed.*, Harper Collins 1993, Pearson, 2006.
2. Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry 3rd Ed.*, John Wiley and Sons, NY, 1994.
3. Basolo, F. & Person, R. *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution 2nd Ed.*, John Wiley & Sons Inc; NY.
4. Purecell, K.F. & Kotz, J.C., *Inorganic Chemistry*, W.B. Saunders Co. 1977
5. Miessler, G. L. & Donald, A. Tarr, *Inorganic Chemistry 4th Ed.*, Pearson, 2010.
6. Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry 4th Ed.*, Wiley India.
7. Collman, James P. et al. *Principles and Applications of Organotransition Metal Chemistry*. Mill Valley, CA: University Science Books, 1987.
8. Crabtree, Robert H. *The Organometallic Chemistry of the Transition Metals*. *j* New York, NY: John Wiley, 2000.
9. Spessard, Gary O., &Gary L. Miessler. *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.

SECTION B-ORGANIC: PHARMACEUTICALS, NATURAL PRODUCTS AND POLYMERS

Unit I: Pharmaceutical Compounds

Structure activity relationship.Classification, structure, mode of action and therapeutic uses of pharmaceutical compounds belonging to the following classes:

1. Analgesics and antipyretics:Paracetamol (synthesis), Ibuprofen (traditional and green synthesis).
2. Antibacterial agents: Sulphonamides. sulphadiazine (synthesis).
3. Antimalarials: Chloroquine (synthesis).
4. Antibiotics: Chloramphenicol (synthesis and structure elucidation).

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

Unit II: Natural Products: Terpenoids and Alkaloids

Terpenoids: Natural occurrence, classification and biosynthesis of terpenoids (with suitable examples including carotenoids).
Structure and specific uses of citral, limonene and α- terpineol.

Alkaloids: Natural occurrence, general methods of Isolation and structural features. (Ziesel's method, Herzig Meyer's method, Hofmann's exhaustive methylation and Emde's modification).
Medicinal importance of nicotine, quinine, morphine and reserpine.

Unit III: Polymers

Polymers: Introduction and classifications.
Polymerisation reactions: Addition, condensation and ring opening metathesis.Polymerisation: Polymerisation: Mechanism of cationic, anionic and free radical addition polymerization, Ziegler-Natta polymerisation of alkenes, stereochemistry of polymers, role of stabilisers, plasticisers, antioxidants, telomers and inhibitors in polymer synthesis.
Preparation from appropriate monomers and applications of following polymers: Polythene, polyvinyl chloride (PVC), polymethylmethacrylate, polyacrylonitrile, polyamides, polyesters, buna-S, neoprene, bakellite and polyurethanes polymers.
Process of vulcanization and its importance.
Introduction to biodegradable, conducting sol-gel and liquid crystal polymers with their importance in day to day life.

Recommended Texts:

1. Morrison, Robert Thornton & Boyd, Robert Neilson *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
3. Finar, I. L. *Organic Chemistry* (*Volume 2: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education) ,Fifth Edition, 1975.
4. Graham Solomons, T.W., Craig B. Fryhle *Organic Chemistry,* Ninth edition John Wiley & Sons, Inc. 2008.
5. Kalsi, P. S. *Textbook of Organic Chemistry 1st Ed.*, New Age International (P) Ltd. Pub. Delete this text
6. Billmeyer, F. W. *Textbook of Polymer Science*, John Wiley & Sons, Inc.
7. Gowariker, V. R.; Viswanathan, N. V. & Sreedhar, J. *Polymer Science*, New age International,First Edition, 1986
8. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry,* Oxford University Press , First Edition, 2001.
9. Singh, J.; Ali, S.M. & Singh, J. *Natural Product Chemistry*, Pragati Parakashan 2010.

PRACTICAL

SECTION A-INORGANIC: PREPARATION OF SELECTED INORGANIC COMPOUNDS AND USE SPECTROSCOPIC TECHNIQUES

i. Measurement of 10 Dq by spectrophotometric method
ii. Verification of spectrochemical series.
iii. Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.
iv. Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+}. Find the λ_{max} of the complex.
v. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

Recommended Texts:

1. Marr. G & Rockett, B.W. Practical Inorganic Chemistry, John Wiley & Sons, 1972.

SECTION-B ORGANIC: EXTRACTION OF NATURAL PRODUCTS, SYNTHESIS OF SELECTED DRUGS AND POLYMERS

1. Extraction of caffeine from tea leaves.
2. Preparation of sodium polyacrylate
3. Preparation of urea formaldehyde.
4. Extraction of active pharmaceutical ingredient from commercial tablet, acetylsalicylic acid from aspirin, its synthesis in laboratory and comparison of the two samples by melting point and TLC.
5. Isolation of ibuprofen and p-acetylaminophenol by solvent extraction from combiflam and their purity analysis by melting point and TLC.
6. Estimation of Vitamin C by titrating it against a solution of 2, 6-dichlorophenol indophenol dye.
7. Quantitative estimation of glucose using Fehling's solution method.

Recommended Texts:

1. Vogel, A.I. *Quantitative Organic Analysis,* Part 3, Pearson 2012.
2. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education 2009.
3. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, *5th Ed.*, Pearson 2012.
4. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis,* University Press 2000.
5. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis,* University Press 2000.

PAPER-16

PHYSICAL: QUANTUM CHEMISTRY, PHOTOCHEMISTRY & SURFACE CHEMISTRY

THEORY

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; wave functions, 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 wave functions. Vibrational energy of diatomic molecules and zero-point energy.

Rigid rotator model of rotation of diatomic molecule.

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 1*s*, 2*s*, 2*p*, 3*s*, 3*p* and 3*d* 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 wave functions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB, only wave functions, detailed solution not required).

Qualitative description of LCAO-MO treatment of second row homonuclear and heteronuclear diatomic molecules (HF, LiH, NO, CO). 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).

Introduction to molecular modelling and geometry optimization (elementary ideas).

Unit II: 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, photosensitized reactions, quenching.

Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence.

Unit III: Surface chemistry

Physical adsorption, chemisorption. Freundlich adsorption isotherm, Langmuir adsorption equation, BET isotherms. Determination of surface area of adsorbent. Gibbs adsorption equation.

Recommended texts:

1. Chandra, A. K. *Introductory Quantum Chemistry*, Tata McGraw-Hill 2001.
2. House, J. E. *Fundamentals of Quantum Chemistry 2nd Ed*., Elsevier: USA 2004.
3. Lowe, J. P. & Peterson, K., *Quantum Chemistry*, Academic Press 2005.
4. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry 8th Ed.*, Oxford University Press 2006.
5. Ball, D. W. *Physical Chemistry*, Cengage, India 2012.
6. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa 2004.
7. Laidler, K. J. *Chemical Kinetics*, Pearson Education: New Delhi 2004.

PRACTICAL

PHYSICAL: MOLECULAR MODELLING

i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.

ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.

iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N_2, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.

iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.

v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 ºC, 100 ºC, 108 ºC, 82 ºC, respectively).

vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.

vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.

viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.

ix. (a) Compare the optimized bond angles H_2O, H_2S, H_2Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

Note: Software: ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer or any similar software.

Recommended Texts:

1. Lewars, E. G. *Computational Chemistry 2nd Ed.,* Springer (India) Pvt. Ltd. 2011, Ch. 1 & 2.
2. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.,* Prentice-Hall 2012, Ch. 26.
3. Rogers, D. W. *Computational chemistry using PC 3rd Ed.,* John Wiley & Sons.

PAPER – 17

RESEARCH METHODOLOGY

THEORY

UNIT I: Introduction to research and General Laboratory Practices:

1. Historical account of research in chemistry.
2. Awareness about material safety data sheet (MSDS), storage, transportation, usages; handling of special chemicals / reagents, such as perchloric acids, formaldehyde, mercury, corrosives, flammables, toxins / poisons, peroxides, labeling of chemicals, Chemical waste.
3. Safety equipments, such as ventilation, fume-hood, fire extinguishers, eye washes, safety showers, first aid kit.
4. Radiation safety: authority, radiation signs & badges and disposal procedure.
5. Biological safety: authority, bio-safety level, pest control, autoclave.
6. Emergency response in case of fire, injury, spills, incident reports, evacuation, emergency contacts, security, excess control, door security, overnight experiments.

UNIT II: Purification Technique and Introduction to Toxic Compounds

1. Purification techniques, drying, distillation and purification of solvents.
2. Types of toxins, such as irritants, corrosives, allergens, asphyxiants, carcinogens, reproductive and development toxins, neurotoxins and their effect on biosystems.

UNIT III: Laboratory-ware and Planning

1. Laboratory equipment handing
2. Maintenance of Laboratory note book, arrangement of analytical data, report-writing, Journal article writing (Abstract, introduction, experimental, results and discussion, conclusion, acknowledgements and references).
3. Planning and execution of laboratory experiments.
4. Product analysis and characterization: physical and spectral analysis.
5. Selection of research topic and its national and international scenario.
6. Uses of various statistical software for structure drawing and graphical representation of data. **Computer Packages:** Applications of some computer packages like MS-Excel, ORIGIN, SciPlot, SciLab, ISIS Draw, ChemSketch. **Introductory writing activities**: Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical and mathematical equations into word processing documents. Using graphs. Presenting data in tables.

UNIT IV: Tools of literature search & literature review.

1. **Print:** Sources of information, Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.
2. **Digital:** Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus.
3. **Information Technology and Library Resources:** The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.

UNIT V: Scientific Writing, Data Analysis and Presentation

1. **The Investigative Approach:** Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments.
2. **Descriptive statistics**: Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, *r* and its abuse. Basic aspects of multiple linear regression analysis.

UNIT VI: Research Ethics and Intellectual property (IP)

Research ethics: Importance, basic principle, authorship, plagiarism, peer review, conflict of interest, data management, research misconduct, ethical issues in living / human subject research **Intellectual property**: History of patent, overview of IP (patents, trademark, copyright, design, trade secrets), Basic definition of Invention, discovery and patent (patentability, infringement), claims and its importance, inventorship vs. authorship.

Recommended Texts:

1. Dean, J. R.; Jones, A. M.; Holmes, D.; Reed, R.; Weyers, J. & Jones, A. *Practical skills in chemistry 2nd Ed.,* Prentice-Hall, Harlow 2011.
2. Hibbert, D. B. & Gooding, J. J. *Data analysis for chemistry*. Oxford University Press 2006.
3. Topping, J. *Errors of observation and their treatment 4th Ed.,* Chapman Hall, London. 1984.
4. Harris, D. C. *Quantitative chemical analysis 6th Ed.,* Freeman 2007, Chapters 3-5.
5. Levie, R. de. *How to use Excel in analytical chemistry and in general scientific data analysis.* Cambridge Univ. Press 2001, 487 pages.
6. Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
7. OSU safety manual 1.01.

PRACTICAL

1. Research Project: To identify a research problems and conduct literature search towards the problem, experimental / computational analysis, data analysis and report writing.
2. Poster making / Paper writing for presentation in scientific conferences / publishers based on above research project.

Recommended Texts:

1. Dawson, C. *Practical Research Methods, A user-friendly guides to mastering research techniques and projects,* 4000 to Books Ltd. 2002.
2. Kothari, C.R. *Research Methodology-methods and Technqiues,* Wiley Eastern Limited, New Delhi 1985.

SEMESTER-VIII

PAPER-18

THEORY

SECTION A- INORGANIC: CHEMISTRY OF INORGANIC SOLIDS, NANOMATERIALS

Unit I: Synthesis and modification of inorganic solids

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

Unit II: Inorganic solids of Technological Importance

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments
Molecular material and fullerides, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystal.

Unit III: Nanomaterials

Preparation of gold and silver metallic nanoparticles, self assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nano tubes and inorganic nanowires. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and antisical nanomaterials, bionano composites.

Recommended Texts:

1. Shriver & Alkins. Inorganic Chemistry, Peter Alkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong, 5th Edition, Oxford University Press (2011-2012)
2. Adam, D. M. Inorganic Solid; An introduction to concepts in solid-state structural chemistry.

SECTION B-PHYSICAL: MOLECULAR SPECTROSCOPY

Unit I: 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.

Recommended Texts:

1. Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy 4th Ed.*, Tata McGraw-Hill: New Delhi 2006.
2. Brown, J. M. *Molecular Spectroscopy*, Oxford Science Publications, New York 1998.

PRACTICAL

SECTION-A INORGANIC: DETERMINATION OF CATION EXCHANGE AND PREPARATION OF NEWER MATERIALS

1. Synthesis of silver nanoparticles and their spectroscopic characterization
2. Preparation and characterization of polyacrylamide hydrogels by the co precipitation method
3. To determine the percentage of tin and lead present in the given amount of solder by complexometric titrimetric procedures.
4. Spectrometric determination of manganese in steel.

Recommended Text:

1. Fahan, *Materials Chemistry*, Springer 2004.

SECTION-B PHYSICAL: UV-VISIBLE SPECTROSCOPY, COLOURIMETRY AND ADSORPTION

UV/Visible spectroscopy

I. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV)

II. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

Colourimetry

I. Determination of dissociation constant of phenolphthalein indicator.

II. Study the kinetics of interaction of crystal violet/phenolphthalein with sodium hydroxide colourimetrically.

Adsorption

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

Recommended Texts:

1. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York 2003.
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York 2003.
4. Sindhu,P.S. *Practicals in Physical Chemistry 1st Ed.* Macmillan: India 2006.

PAPER-19

ORGANIC: CHEMISTRY OF BIOMOLECULES

THEORY

Unit I: Amino acids, Peptides and Proteins

Amino acids: Classification, relative and absolute configuration.
Synthesis of α-Amino acids: Phthalimide synthesis, Strecker synthesis, phthalimidomalonic ester synthesis and azalactone synthesis.
Ionic properties and reactions: Zwitter ions, pKa values, isoelectric point, application of electrophoresis (gel and paper) and ion exchange chromatography in separation and purification of amino acids and proteins.
Peptides: Peptide linkage, determination of their primary structures, end group analysis (Edmans, Sanger's and Dansyl chloride method only), application of partial hydrolysis (chemical, enzymatic). Peptide synthesis: using N-protecting groups (Boc and benzyloxycarbonyl methods only), *C*-protecting group, *C*-activating groups (acid chloride, acid azide, activated esters and DCC methods only) and Solid-phase synthesis.
Proteins: classification, tests in laboratory and biological importance, primary, secondary(α-helix and β- pleated sheets), tertiary and quaternary structures of proteins.

Unit II: Enzymes

Introduction, classification and characteristics of enzymes. Salient features of active site of enzymes.
Mechanism of enzyme action(taking trypsin as example), factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive , uncompetitive and non-competitive inhibition including allosteric inhibtion).

Unit III: Lipids

Lipids: Introduction and classification.
Oils and fats : Common fatty acids present in oils and fats, essential fatty acids and their importance, omega fatty acids, trans fats, hydrogenation, saponification value, iodine number, acid number, drying, rancidity (hydrolytic and oxidative) and reversion.
Biological importance of triglycerides, phospholipids, glycolipids, sphingolipids and steroids (cholesterol). Liposomes and their biomedical applications.

Unit IV: Nucleic Acids

Components of nucleic acids: Nitrogenous bases (adenine, guanine, thymine, uracil and cytosine), sugar and phosphate; nucleosides, nucleotides and their nomenclature; Phosphodiester linkage and structure of polynucleotides; structure of DNA (Watson-Crick model) and RNA(types of RNA), genetic code.
Biological roles of DNA and RNA: Introduction to replication, transcription and translation.

Unit V: Concept of Energy in Biosystems

Cells obtain energy by the oxidation of foodstuff (organic molecules).
Introduction to metabolism (catabolism, anabolism).
ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change.
Agents for transfer of electrons in biological redox systems: NAD^+, FAD.
Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle.
Overview of catabolic pathways of fat and protein.
Interrelationship in the metabolic pathways of protein, fat and carbohydrate.
Caloric value of food, standard caloric content of food types.

Recommended Texts:

1. Morrison, Robert Thornton & Boyd, Robert Neilson *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Sixth Edition, 2003.
3. Finar, I. L. *Organic Chemistry* (*Volume 2: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), Fifth Edition, 1975.
4. Graham Solomons, T.W., Craig B. Fryhle *Organic Chemistry*, Ninth edition John Wiley & Sons, Inc. 2008.
5. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, Oxford University Press, First Edition, 2001.
6. Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Bioch*emistry, Fifth Edition, 2010., W. H. Freeman.
7. Berg, J. M.; Tymoczko, J. L. & Stryer, L. *Biochemistry*, Seventh Edition, 2012., W. H. Freeman.

PRACTICAL

ORGANIC: ISOLATION AND ESTIMATION OF SELECTED BIOMOLECULES AND PREPARATION OF ORGANIC COMPOUNDS

1. Estimation of phenol and aniline by bromination with potassium bromated-potassium bromide method.
2. Estimation of glycine by Sorenson's formalin method.
3. Study of the titration curve of glycine.
4. Estimation of proteins by Lowry's method.
5. Study of the action of salivary amylase on starch at optimum conditions.
6. Effect of temperature on the action of salivary amylase.
7. Saponification value of an oil or a fat.
8. Determination of Iodine number of an oil/fat.
9. Isolation and characterization of DNA from onion/cauliflower/peas.

Recommended Texts:

1. Mannual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.
2. Arthur, I. V. *Quantitative, Organic, Analysis s* Pearson.
3. Cooper, T.G. *The Tools of Biochemistry,* John Wiley and Sons, N.Y. USA. 16 (1977).

PAPER-20

RESEARCH

Dissertation based on Research: Suitable Topics in Chemical Sciences

Presentation & Viva-voce

1. Students will be divided among faculty members of the Department for the supervision of the research work. For example- if there are 50 students and five faculty members, each member will be assigned 10 students for supervision.
2. In the first week of Semester VII, each faculty member will assign a suitable research topic to the students from the selected topics in the areas of chemical sciences.
3. The student will work on the assigned research topic during semesters VII and VIII in regular consultation with his/her assigned teacher.
4. The student will write a dissertation based on the research work carried out during Semesters VII and VIII and prepare two copies to be submitted to the office of the Principal of the college duly signed by the student and the supervisor in the last week of VIII semester.
5. The office of the Principal will take a note of the submission of the dissertation and return the copies each to the student and the teacher for examination.
6. The student will make a power point presentation based on the work carried out and mentioned in the dissertation to the board of examiners appointed by the University.

DC –II CHEMISTRY

SEMESTER -III

PAPER – 1

CHEMICAL BONDING

Knowledge of Inorganic compounds is very important to most of the Scientists involved in different fields of Chemistry and in all other Sciences. This paper will help the student understand and rationalize the bonding in compounds, the basic shapes and structures of molecules in gaseous and solid state and even predict properties which may be of potential interest to their use as materials. Geology, Environmental Science, Molecular Biology, Material and Polymer Science, require knowledge of these Inorganic compounds (materials). This would prepare a strong and an essential base for them to integrate chemistry with their discipline at higher level.

THEORY

Unit 1: The Covalent Bond and the structure of molecules

Valence Bond Approach , Concept of Resonance in various Organic and Inorganic compounds, hybridisation and structure, Equivalent and non-equivalent hybrid orbitals, Bent's rule and its applications ,VSEPR model for predicting shapes of molecules and ions containing lone pairs, sigma and pi bonds

Unit 2: Molecular Orbital Approach

LCAO method, symmetry and overlap for s-s ,s-p and p-p combinations, MO treatment of homonuclear diatomic molecules of 2^{nd} period (B_2, C_2 ,N_2, O_2 ,F_2) and heteronuclear di-atomic molecules (CO ,NO) and their ions.

Unit 3: Bonding in Solid State

The close packing of atoms and ions in solids , size effects of atoms and ions, Fajan's rule (atomic and
ionic radius ratio in crystalline solids) and isomorphous subsitutions.
Lattice energy (Born-Haber cycle) .
Stoichiometric and non-stoichiometric defects in Solids , Solid solutions and alloys.
Band theory (conductors, semi-conductors and insulators).

Unit 4: Intermolecular forces:

van-der Waals forces, Hydrogen bonding and its applications, effect of these forces on melting point, boiling point and solubility.

Suggested Texts:

1. James E. Huheey, *"Inorganic Chemistry: Principles of structure and reactivity"*, Pearson Education, IV Edition 2006.
2. D. S. Shriver and P.A. Atkins, *"Inorganic Chemistry"*, Oxford University Press, V Edition 2009.
3. Alan G. Sharpe, "*Inorganic Chemistry"*, Pearson Education, III Edition 1981.
4. J. D. Lee, *Concise Inorganic Chemistry*, John Wiley & Sons, NY, V Edition 2008.
5. Grey L. Miessler and Donald A. Tarr, *"Inorganic Chemistry"*, Prentice Hall, IV Edition 2011.
6. B. Douglas, D. H. McDaniel and J. J. Alexander, *"Concepts and Models of Inorganic Chemistry",* John Wiley and Sons, III Edition 1994.

PRACTICAL

TITRIMETRIC ANALYSIS

Preparations of standard solutions (concept of primary and secondary standards), Different units of concentration (molarity, molality, normality and formality)

(A) Titrations involving acids-Bases:

Principle of acid-base titrations, Principle behind selection of an appropriate indicator.

i. Standardization of NaOH solution (standard solution of oxalic acid to be prepared)
ii. Determination of concentration of carbonate and hydroxide present in a mixture.
iii. Determination of concentration of carbonate and bicarbonate present in a mixture.
iv. Determination of concentration of free alkali present in soaps/detergents/shampoos.

(B) Titrations involving redox reactions:

Concept of electrode potential, principle behind selection of an appropriate indicator.

i. Standardization of $KMnO_4$ solution (standard solution of Mohr's salt to be prepared).
ii. Determination of concentration of Fe (II) in Mohr's salt and/or $K_2Cr_2O_7$ using diphenylamine / N-phenylanthranilic acid as internal indicator (standard solution of $K_2Cr_2O_7$ and /or Mohr's salt to be prepared).
iii. Determination of iron content in ores / alloys using appropriate redox titration.

Recommended Texts:

1. *Vogel's Textbook of Quantitative Inorganic Analysis*, John Wiley & Sons, NY, V Edition1989.
2. Harris, D.C. *Quantitative Chemical Analysis,* Freeman, W.H. & Co.Inc.NY, VII Edition, 2007**.**

SEMESTER-IV

PAPER-2

CONCEPTUAL ORGANIC CHEMISTRY

Organic chemistry is the chemistry of carbon compounds and is probably the most active and important field of chemistry, due to its extreme applicability to both, life and industry. Organic chemistry involves few basic principles and many extensions and applications of these principles. After studying this paper one gets an insight of these principles. Many reactions would be discussed which are used in day to day life . Three dimentional structures of organic molecules will also be covered in this paper.

THEORY

Unit 1: Stereochemistry

Writing of Fischer projection, Newmann and Sawhorse projection and Wedge formulae.Interconversion of one type of structural representation into another type of formulae.

Conformations : Restricted rotation about single bonds, Various conformations of ethane, butane , ethane-1,2-diol and cyclohexane . Relative stability of different conformations in terms of energy difference is to be discussed for all these compounds .

Geometrical Isomerism :Requirements for a molecule to show geometrical isomerism, Cis-Trans and E/ Z notation along with CIP rules for naming geometrical isomers.

Optical Isomerism : Optical activity, specific and molar rotation, chirality, enantiomerism, diastereoisomerism, racemic mixtures and their resolution by salt formation method.

Relative and absolute configuration: D / L nomenclature system for configuration of carbohydrates (difference between d/l and D/L notations) .Threo and Erythro designation. R- and S- configuration (upto two chiral centers).

Unit 2: Addition Reactions

Alkenes and Alkynes : Hydrogenation, addition of halogens ,Hydrohalogenation (Markovnikov's and antiMarkovnikov's addition) ,hydration,hydroxylation (cis and trans), oxymercuration-demercuration , hydroboration-oxidation, ozonolysis. Reactivity of alkenes vs alkynes.

Aldehydes and ketones : (formaldehyde, acetaldehyde, benzaldehyde, acetone)

Addition of sodium bisulphite,hydrogen cyanide and alcohols.

Addition- elimination reactions with ammonia and its derivatives

Name reactions :Aldol, cross Aldol, Claisen, Knoevenagel, Cannizzaro, cross Cannizzaro

Unit 3: Substitution Reactions

Free radical substitution reactions: Halogenation of alkanes, allylic compounds and alkyl benzenes.
Nucleophilic substitution reactions: Alkyl, allyl and benzyl halides – substitution of halogen by some common nucleophiles. mechanism of S_N1 and S_N2 reactions (stereochemistry, nature of substrate, nucleophile and leaving group)
Benzene diazoniumchloride: replacement of diazo group
Alcohols,amines and phenols: substitution of active hydrogen, replacement of hydroxyl group in alcohols (using PCl_5, $SOCl_2$ and HI)
Carboxylic acid derivatives: hydrolysis
Ethers: cleavage by HI
Electrophilic Substitution Reactions (aromatic compounds) : General mechanism of electrophilic substitution reactions (nitration,halogenation, sulphonation,Friedel Crafts alkylation and acylation), directive influence of substituents .

Unit 4: Elimination Reactions

Alkyl halides (dehydrohalogenation, Saytzeff's rule), vicinal dihalides (dehalogenation), alcohols (dehydration) , Quaternary ammonium salts (Hofmann's elimination). Mechanism of E1 and E2 reactions (nature of substrate and base) , elimination vs substitution

Unit 5: Oxidation

Aromatic side chain : oxidation with potassium permanganate, potassium dichromate
Alcohols :oxidation with potassium permanganate, potassium dichromate, catalytic dehydrogenation and Oppenauer oxidation. Oxidation of 1,2 –diols with periodic acid and lead tetraacetate.
Aldehydes : oxidation with potassium permanganate, chromic acid and Tollen's reagent
Ketones : oxidation with potassium permanganate, sodium hypoiodite(iodoform reaction) and Baeyer – Villiger oxidation

Unit 6: Reductions

Aldeydes and ketones : catalytic hydrogenation, reduction with sodium borohydride, lithium aluminium hydride, Clemmensen,and Wolff-Kishner reduction.
Carboxylic acids and their derivatives : Lithium aluminium hydride, sodium-ethanol and Rosenmund reduction.
Nitro compounds : Acidic , alkaline and neutral reducing agents, lithium aluminium hydride and electrolytic reduction.

Recommended Texts:

1. I. L. Finar : *Organic Chemistry* (Vol. I & II), Pearson Education,VI Edition, 1973.

2. R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Pearson Education,VI Edition, 1992,
3. Arun Bahl and B. S. Bahl : *Advanced Organic Chemistry*, S. Chand & Co. Ltd. III Edition, 1987.
4. Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry,* Pearson Education, VI Edition, 2003.
5. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*; Wiley: London, 1994.
6. T. W. Graham Solomon's :*Organic Chemistry,* John Wiley and Sons, IX Edition, 2008
7. P.S. Kalsi,*Stereochemistry,Conformation and Mechanism,* New Age International Publishers,VII Edition, 2008.
8. D.Nasipuri, *Stereochemistry of Organic Compounds,* New Age International Publishers 2011.

PRACTICAL

PURIFICATION OF ORGANIC COMPOUNDS AND ORGANIC PREPARATION AND RELATED REACTIONS

1. Purification of organic compounds by crystallization using the following solvents:
    a. Water
    b. Alcohol
2. Determination of the melting points of organic compounds (by Kjeldahl method and electrically heated melting point apparatus).
3. Determination of optical activity by using polarimeter
   Organic preparations : Carry out the following preparations using 0.5-1 g. of starting compound. Recrystallize the product and determine the melting point of the recrystallized sample.
4. To prepare acetanilide by the acetylation of aniline.
5. To prepare p-bromoacetanilide.
6. Benzolyation of aniline or β-naphthol by Schotten-Baumann reaction
7. Hydrolysis of benzamide or ethyl bezoate.
8. Semicarbazone derivative of one the following compounds: acetone, ethyl methyl ketone, diethylketone, cyclohexanone, benzaldehyde.
9. Nitration of nitrobenzene.
10. Oxidation of benzaldehyde by using alkaline potassium permanganate.

Recommended Texts:

1. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, Pearson Education, V edition 2012.
2. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry,* Longman, London & New York, IV Edition 2009.
3. Ahluwalia, V.K.; Dhingra, S. & Gulati, A. *College Practical Chemistry,* Universities Press 2005.

SEMESTER-V

PAPER-3

THERMODYNAMICS, EQUILIBRIUM IN CHEMISTRY AND ELECTROCHEMISTRY

It is important to understand the forces which drive the chemical reactions in forward direction and the concept of the interchange of energy in a system. This paper also discusses the use of electrical energy for initiating chemical reactions and also how chemical reactions can be utilized to produce electrical energy. The basic principle used in the formation of cells and battries would also be taken up.

THEORY

Unit 1: Thermodynamics

State of a system, state variables, intensive and extensive variables, concept of heat and work, thermodynamic equilibrium,

First Law of thermodynamics. Calculation of work (w), heat (q), changes in internal energy (ΔU) and enthalpy (ΔH) for expansion or compression of an ideal gas under isothermal conditions for both reversible and irreversible processes. Calculations of w, q, ΔU and ΔH for processes involving changes in physical states. Laws of thermochemistry, enthalpy of combustion, enthalpy of neutralization and integral enthalpies of solution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Kirchhoff's equation.

Statements of Second Law of thermodynamics, concept of entropy, Gibbs energy and Helmholtz energy, criteria of spontaneity. Gibbs–Helmholtz equation.

Statement of Third Law of thermodynamics and calculations of absolute entropies of substances.

Unit 2: Chemical Equilibrium

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔG^{o}, Qualitative treatment of Le Chatelier's principle. Relationships between K_p, K_c and K_x.

Unit 3: Ionic Equilibrium

Strong and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water, pH scale. Ionization of weak acids and bases, common ion effect, Salt hydrolysis and simple calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions, buffer capacity and buffer range. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

Unit 4: Electrochemistry

Metallic and electrolytic conductance, conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions.Concept of transference number. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, conductometric titrations (acid-base).
Reversible and irreversible cells. Concept of EMF of a cell, measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes, standard electrode potential, electrochemical series. Thermodynamics of a reversible cell. Calculation of equilibrium constant of a cell reaction from EMF data.

Recommended Texts:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* , Oxford University Press IX Edition 2011.
2. Ball, D. W. *Physical Chemistry* Thomson Press, India 2007.
3. Castellan, G. W. *Physical Chemistry* , Narosa, IV Edition 2004.
4. Mortimer, R. G. *Physical Chemistry* , Elsevier: Noida, UP, III Edition 2009.

PRACTICAL

THERMOCHEMISTRY, POTENTIOMETRIC AND CONDUCTOMETRY

(I) Thermochemistry

1. Determination of heat capacity of a calorimeter for different volumes.
2. Determination of the enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of integral enthalpy of solution of salts (endothermic and exothermic).

(II) pH and potentiometric measurements

4. Preparation of sodium acetate-acetic acid buffer solutions and measurement of their pH.
5. Potentiometric titrations of (i) strong acid *vs* strong base (ii) weak acid *vs* strong base
6. Determination of dissociation constant of a weak acid.

(III) Conductometry

7. Conductometric titrations of (i) strong acid-strong base (ii) weak acid-strong base.

Recommended Texts:

1. Khosla, B.D.; Garg, V.C.; Gulati, A. & Chand, R. *Senior Practical Physical Chemistry*, New Delhi, 1985.
2. Sindhu, P.S. *Practicals in Physical Chemistry,* Macmillan India Ltd. 2005.

SEMESTER-VI

PAPER-4

COORDINATION CHEMISTRY AND BIO-INORGANIC CHEMISTRY

Transition metal complexes play an important role in Inorganic Chemistry. The objective of Unit I in this paper is to introduce the structure and bonding theories, electronic and magnetic properties of the transition metal complexes and their kinetic studies. Theories of bonding in Coordination compounds explain their experimental behaviour. It imparts a working knowledge of Coordination Chemistry and its importance. It bridges the gap between Chemistry and Physics.

Bioinorganic Chemistry is the study of the 'Inorganic" elements in biological systems. The objective of Unit II in this paper is to understand the interaction of metal ions with biological ligands. It explains the role of Inorganic "substances" in living systems and the use of metal ions in medicinal therapy and diagnosis. It bridges the gap between Inorganic Chemistry and Biochemistry.

THEORY

Unit 1: Coordination Chemistry

Crystal Field Theory: Shapes of d-orbitals, Crystal field splitting in Octahedral and Tetrahedral complexes. Measurement of 10 Dq and Crystal Field Stabilization energy in Weak and Strong Fields. Pairing Energies. Octahedral vs. Tetrahedral Coordination. Tetragonal Distortions from Octahedral Symmetry. The Jahn – Teller Theorem. Square Planar coordination. Factors affecting the Magnitude of 10 Dq. Spectrochemical series. Applications of CFT: Special reference to colour of the metal complexes, Magnetic properties of the metal complexes, Consequences of Crystal field splitting – Variation in ionic radii, Lattice energy, Hydration energy and structures of mixed oxides of spinel type etc

Stability of metal complexes: Stepwise formation constants, the difference between the Thermodynamic and Kinetic stability,Chelate Effect, Labile and Inert Complexes.. The Trans Effect. Mechanism of the Trans Effect..

Unit 2: Bioinorganic Chemistry

Metal ions present in biological systems, classification of elements as essential, non-essential, trace and toxic. Bioinorganic chemistry of toxic metals—lead, cadmium, mercury and arsenic. Mechanism of toxicity and. Detoxification using chelating agent. Bioinorganic chemistry of platinum- anticancer drug.

Role of iron in human system with reference to Haemoglobin and Myoglobin. Perutz mechanism for oxygenation of Haemoglobin. Role of globin in Haemoglobin. Cooperative effect. Role of alkali and alkaline earth metals((sodium,potassium,calcium and magnesium) in biological system.(Sodium-Potassium pump).

Recommended Texts:

1. J. D. Lee, *Concise Inorganic Chemistry*, John Wiley & Sons, NY, V Edition, 2008.
2. James E. Huheey, *"Inorganic Chemistry: Principles of structure and reactivity"*, Pearson Education, IV Edition 2006.
3. Gary L. Miessler & Donald A. Tarr, Pearson, "*Inorganic Chemistry*", Prentice Hall Publishers.
4. D. S. Shriver & P. A. Atkins, *Inorganic Chemistry*, Oxford University Press. II Edition, 1994.
5. S. J. Lippard, & J. M. Berg, *Principles of Bioinorganic Chemistry* Panima Publishing Company, 1994.
6. R. R. Crichton, *Biological Inorganic Chemistry, An Introduction*, Elsevier 2012.
7. J. M. Berg, J. L. Tymoczko & L. Stryer, *Biochemistry*, W. H.Freeman, V Edition, 2002.

PRACTICAL

SELECTED INORGANIC TITRATIONS AND RELATED REACTIONS

1. Determination of concentration of Mg (II) & Zn (II) by titrimetric method using EDTA.
2. Determination of concentration of Ca (II) in solution by (substitution method) using Eriochrome Black T as an indicator.
3. Determination of concentration of Ca/Mg in drugs or in food samples.
4. Determination of concentration of total hardness of a given sample of water by complexometric titration.
5. Preparation of Tetraamminecopper(II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$.
6. Preparation of Potassium tris(oxalato)chromate(III), $K_3[Cr(C_2O_4)_3]$.
7. Determination of concentration of Na^+, K^+, Ca^{2+} and Mg^{2+} using flame photometry.
8. To draw the calibration curve (absorbance at λ_{max} vs. concentration) for various concentrations of a given coloured compound and estimate the concentration of the same in a given solution.
9. Determination of composition of the Fe^{2+}-1,10-phenanthroline/Fe^{3+}-salicyclic acid complex in solution by Job's method.

Recommended Texts:

1. Khosla, B.D.; Garg, V.C.; Gulati, A. & Chand, R. *Senior Practical Physical Chemistry*, New Delhi 1985.
2. Sindhu, P.S. *Practicals in Physical Chemistry,* Macmillan India Ltd. 2005.

SEMESTER-VII

PAPER- 5

MOLECULES OF LIFE

It is the harmonious and synchronous progress of chemical reactions in body which leads to life.These chemical reactions involve certain molecules called biomolecules or molecules of life. These molecules constitute the source of energy in body, build the body, act as catalyst in many processes and also responsible for the transefer of characters to offsprings. In this paper one would get the information about the structures of these molecules and their role in life related processes. The basic types of molecules included are carbohydrates, proteins,enzymes, lipids and nucleic acids.

THEORY

Unit 1: Carbohydrates.

Classification of carbohydrates, reducing and non reducing sugars, General Properties of Glucose and Fructose ,their open chain structure. Epimers, mutarotation and anomers. Determination of configuration of Glucose (Fischer proof).
Cyclic structure of glucose . Haworth projections. Cyclic structure of fructose.
Linkage between monosaccharides, structure of disaccharides (sucrose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

Unit 2: Amino Acids, Peptides and Proteins

Classification *of* Amino Acids,Zwitter ion structure and Isoelectric point.
Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins. Determination of Primary structure of Peptides ,determination of N-terminal amino acid
(by DNFB and Edman method) and C–terminal amino acid(by thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid phase synthesis.

Unit 3: Enzymes and correlation with drug action

Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, Specificity of enzyme action(Including stereospecifity), Enzyme inhibitors and their importance, phenomenon of inhibition(Competitive and Non competitive inhibition including allosteric inhibtion). Drug action-receptor theory. Structure – activity relationships of drug molecules,binding role of –OH group,-NH_2 group, double bond and aromatic ring,

Unit 4: Nucleic Acids

Components of Nucleic acids: Adenine, guanine ,thymine and Cytosine(Structure only), other components of nucleic acids, Nucleosides and nucleotides**(nomenclature**), Structure of polynucleotides; Structure of DNA (Watson-Crick model) and RNA(**types of RNA**), Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation.

Unit 5: Lipids

Introduction to lipids , classification.
Oils and fats : Common fatty acids present in oils and fats, Omega fatty acids, Trans fats,Hydrogenation, Saponification value, Iodine number.
Biological importance of triglycerides, phospholipids, glycolipids, and steroids (cholesterol).

Unit 6: Concept of Energy in Biosystems

Calorific value of food. Standard caloric content of carbohydrates, proteins and fats.
Oxidation of foodstuff (organic molecules) as a source of energy for cells. Introduction to Metabolism (catabolism, anabolism) , ATP: the universal currency of cellular energy,
ATP hydrolysis and free energy change.
Conversion of food into energy. Outline of catabolic pathways of Carbohydrate- Glycolysis, Fermentation, Krebs Cycle. Overview of catabolic pathways of Fats and Proteins. Interrelationships in the metabolic pathways of Proteins,Fats and Carbohydrates.

Recommended Texts:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Pearson Education, VI Edition, 1992.
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Pearson Education,VI Edition, 1973.
3. Finar, I. L. *Organic Chemistry* (*Volume 2)*, Pearson Education, VI Edition, 1973.
4. Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Bioch*emistry , W. H. Freeman VII Edition, 2004.
5. Berg, J. M., Tymoczko, J. L. & Stryer, L. *Biochemistry,* W. H. Freeman, V Edition, 2002.

PRACTICAL

EXTRACTION, SEPARATION AND PURIFICATION OF SELECTED BIOMOLECULES & DRUGS

1. Separation of aminoacids by paper chromatography
2. To determine the concentration of glycine solution by formylation method.
3. Study of titration curve of glycine
4. Action of salivary amylase on starch
5. Effect of temperature on the action of salivary amylase on starch.
6. To determine the saponification value of an oil/fat.
7. To determine the iodine value of an oil/fat
8. Differentiate between a reducing/nonreducing sugar.
9. Extraction of DNA from onion/cauliflower

10. To synthesise aspirin by acetylation of salicylic acid and compare it with the ingredient of an aspirin tablet by TLC.

Recommended Texts:

1. Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. *Vogel's Textbook of Practical Organic Chemistry*, ELBS.
2 Ahluwalia, V.K.; Dhingra, S. & Gulati, A. *College Practical Chemistry*, Universities Press, 2005.

SEMESTER-VIII

PAPER-6

QUANTUM CHEMISTRY & SPECTROSCOPY, PHASE EQUIBRIUM, CHEMICAL KINETICS AND PHOTO CHEMISTRY

This paper deals with the quantum chemistry and quantization of energy. The atomic structure is better understood by the concept of quantization of energy of different orbitals . The absorption of energy by the molecules, produces spectra which help in structure determination and identification of the molecules .This energy can initiate the photo-chemical reactions which would also be discussed in this paper. Phase equilibria help in understanding the formation of various materials, allotropic forms of different substances.

THEORY

Unit 1: Quantum Chemistry and spectroscopy

Postulates of quantum mechanics, quantum mechanical operators.
Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wavefunctions, concept of zero-point energy and Heisenberg Uncertainty principle; wavefunctions, probability distribution functions, nodal properties. Average position.
Qualitative treatment of hydrogen atom and hydrogen-like ions, central field problem, quantization of energy (only final energy expression), radial part of wave function. Average distance of electron from the nucleus.
Spectroscopy and its importance in chemistry. Link between quantum chemistry and spectroscopy. Electromagnetic radiation and its interaction with matter. Types of spectroscopy. Difference between atomic and molecular spectra. Born-Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components.
Rotational spectroscopy: Quantization of rotational energy levels (only expression), selection rules, intensities of spectral lines, determination of bond lengths of diatomic molecules.
Vibrational spectroscopy: Quantization of vibrational energy levels (only expression), selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules.

Unit 2: Phase Equilibrium

Phases, components and degrees of freedom of a system. Gibbs phase rule for non reactive system, derivation of Clausius – Clapeyron equation and its importance in phase equilibria.
Phase diagrams of one-component systems (water and sulphur)
Binary solutions:Partially miscible liquids, immiscible liquids,steam distillation.
Nernst Distribution law and its application in solvent extraction

Unit 3: Chemical Kinetics

The concept of reaction rates. Effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero and first order reactions. Half–life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation.

Unit 4: Photochemistry

Laws of photochemistry. Lambert-Beer's law. Fluorescence and phosphorescence. Quantum efficiency and reasons for high and low quantum yields. Primary and secondary processes in photochemical reactions. Photochemical and thermal reactions.

Recommended Texts:

1. Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy,* Tata McGraw-Hill: New Delhi, IV Edition, 2006.
2. Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill, 2001.
3. House, J. E. *Fundamentals of Quantum Chemistry* Elsevier, II Edition, 2004.

PRACTICAL

STUDY OF KINETICS OF THE REACTIONS, COLOURIMETRY AND PHASE DIAGRAM

(I) Study of the kinetics of the reactions.

1. Initial rate method: Iodide-persulphate reaction
2. Integrated rate method:
   a. Acid hydrolysis of methyl acetate with hydrochloric acid.
   b. Saponification of ethyl acetate

(II) Colourimetry

3. Verification of Lambert-Beer's Law for potassium dichromate/ potassium permanganate/copper sulphate solution.
4. Determination of pK (isndicator) for phenolphthalein.
5. Study the kinetics of interaction of crystal violet with sodium hydroxide colourimetrically.

(III) Phase diagram

6. Phase diagram of phenol-water system.

Recommended Texts:

1. *Vogel's Textbook of Quantitative Inorganic Analysis*, John Wiley & Sons, NY, V Edition1989
2. Harris, D.C. *Quantitative Chemical Analysis* , Freeman, W.H. & Co.Inc.NY , VII Edition, 2007**.**

SYLLABUS FOR APPLIED CHEMISTRY

SEMESTER-III

COMPUTER APPLICATIONS IN CHEMISTRY

100 Marks

Computers have taken a very important role in our daily life and are being used by chemistry students extensively all over the world. Both the programming as well as the application software aspects is quite useful for Chemistry students. The undergraduate curriculum covers the programming language QBASIC which is good for the beginners. It also deals with an application software like ChemSketch that helps students to write chemical reactions and to draw structures, etc.

Basic Computer system:

Operating Systems (DOS, WINDOWS, and Linux); Software languages: Low level and High level languages (Machine language, Assembly language; QBASIC, FORTRAN and C++); Software products (Office, ChemDraw/ Chemsk11), internet applications.

Programming Language – QBASIC/GWBASIC/qb64

QBASIC Commands: INPUT and PRINT Commands; GOTO, IF, ELSEIF, THEN and ENDIF Commands; FOR and NEXT Commands; Library Functions (ABS, ASC, CHR$, EXP, INT, LOG, RND, SQR, TAB and trigonometric functions), DIM, READ, DATA, REM, RESTORE, DEF FN, GOSUB, RETURN, SCREEN, VIEW, WINDOW, LINE, CIRCLE, LOCATE, PSET Commands.

BASIC programs for solution of quadratic equation, polynomial equations (iterative and Newton–Raphson methods) and numerical integration (Trapezoidal rule, Simpson's rule).

Use of Computers for Solving Problems in Chemistry

The above commands/ keywords of QBASIC/ GWBASIC/ qb64 *may be used for solving simple chemistry numerical/ graphical problems. Some of the <u>suggested</u> exercises are (encourage new and innovative exercises in chemistry):*

1. (a) Calculate the pressure of a gas using the ideal gas equation, van der Waals equation, Dietrici equation, and Berthelot equation. (b) Compare the results.
2. Find the root mean square, average and most probable velocities of a gas at different temperatures.
3. Compute w, q, ΔU, and ΔH of three mol of an ideal gas expanded isothermally from 20 dm^3 to 60 dm^3 in the two processes: (i) Irreversible expansion against constant opposing pressure of 100 kPa, and (ii) Reversible process at a fixed temperature of 27 °C.

4. Calculate ΔH and ΔS for an isothermal increase in pressure of CO_2 from 0.1 MPa to 10.0 MPa assuming van der Waals behaviour; a = 0.366 m^6 Pa mol^{-1}, $b = 42.9\times10^{-6}$ m^3 mol^{-1} at 300 K and 400K and compare with the ideal gas values.
5. Calculate the energy of the ground level of an electron with mass 10^{-30} kg in a box the size of an atom, 10^{-10} m. Compare it with that in a box the size of the nucleus, 10^{-14} m. Also calculate the coulombic energy that holds the electron in the nucleus.
6. Find the activation energy for the decomposition of HI if the activation energy for the reaction $H_2 + I_2 \rightarrow 2$ HI is 167 kJ and the ΔE for the reaction is -8.2 kJ.
7. Calculate the pressure of nitrogen gas as a function of height using the ideal gas equation. Also plot the ratio of p/p_0 versus the height of the column at three different temperatures. p_0 is the pressure of the gas at the bottom of the column.
8. Plot the wave functions and probability densities for the particle in a 1-D box system.
9. Solve the quadratic equation and thus find the pH value of 0.001 M HCl and 10^{-8} M HCl solutions by (a) direct solution (b) simple iteration or (c) Newton –Raphson iteration.
10. Plot a pH metric titration curve for a weak acid, acetic acid, with a strong base, sodium hydroxide.
11. Plot the experimental data of miscibility temperature versus composition for (a) phenol-water system (b) triethylamine – water system.
12. Calculate the dissociation energy of I_2 using the electronic–vibration transitions ΔE vs v data (numeric integration by Trapezoidal rule/ Simpson's rule)..
13. Write a program for solution of the quadratic equation $ax^2 + bx + c = 0$ and calculate pH value of 10^{-8} M HCl solution.
14. Wri*te* a program to find the value of a determinant and calculate eigen value.
15. Write a program for solution of a cubic equation and calculate molar volume of a gas using van der Waals equation.

Recommended Texts:

1. Microsoft GW-BASIC Operating System User's Guide.
2. Holmes, B. J. *BASIC programming*. Galgotia Booksource 1986.
3. Balagurusamy, E. *BASIC programming 3rd Ed*., Tata McGraw-Hill 2001**.**
4. Gottfried, B. S. *Schaum's Outline Series: Theory and Problems of Programming with BASIC* McGraw-Hill 1986.
5. Lotia, M.; Nair, P. & Lotia, P. *Modern all about GW-BASIC* BPB Publications: New Delhi 1995.
6. Kapoor, K. L. *A Text-book of Physical Chemistry. Vol. 6* Macmillan 2010.
7. Sinha, P. K. *Computer Fundamentals* BPB Publications: New Delhi 2004.
8. Rajaraman, V. *Fundamentals of Computers* PHI Learning Pvt. Ltd. 2003.
9. Balagurusamy, E. *Fundamentals of Computers* Tata McGraw-Hill: New Delhi 2009.
10. Mortimer, R. G. *Mathematics for Physical Chemistry 3rd Ed.*, Academic Press: 2005.

SEMESTER-IV

ANALYTICAL CHEMISTRY

100 Marks

Analytical Chemistry forms thse back bone for the research in academics as well as in industries. Human resource equipped with up to date analytical skills from reputed universities fall short of demand. With the advancement in technological innovation, the need to create more manpower falls under the discipline of emerging area.

Analytical Chemistry deals with the detection, identification separation, and estimation of atomic, molecular, and ionic species in various states.

1. **Introduction:** Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation of experimental data and results, from the point of view of Significant figures.

2. **Analysis of soil**: Composition of soil, Concept of pH and pH measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators
    a. Determination of pH of soil samples.
    b. Estimation of calcium and magnesium ions by complexometric titrations and flame photometry wherever applicable.

3. **Analysis of water:** Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.
    a. Determination of pH, acidity and alkalinity of a water sample.
    b. Determination of dissolved oxygen (DO) of a water sample.

4. **Analysis of food products:** Nutritional value of foods, idea about food processing and food preservations and adulteration.
    a. Identification of adulterant in some common food items like coffee powder, asafetida, Chilli powder, Turmeric powder, Coriander powder and Pulses etc.
    b. Analysis of preservatives and colouring matter.

5. **Chromatography:** Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.
    a. Paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}).
    b. To compare paint samples by TLC method.

6. **Ion-exchange chromatography**: Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

7. **Analysis of cosmetics:** Major and minor constituents and their function
    a. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
    b. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

8. **Spectrophotometric demonstrations:**
    a. Determination of an equilibrium constant and pKa value for an acid-base indicator.
    b. Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.
    c. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drink.

Suggested Texts:

1. Willard, H. H. *Instumental Methods of Analysis*, CBS Publishers 1992.
2. Skoog & Lerry. *Instrumental Methods of Analysis*, Saunders College Publications, New York, 1985.
3. Skoog, D.A.; West, D.M. & Holler, F.J. *Fundamentals of Analytical Chemistry 6th Ed.*, Saunders College Publishing, Fort Worth 1992.
4. Harris, D. C. *Quntitave Chemical Analysis 7th Ed.*, W. H. Freeman and Company, Inc. NY, 2007 .
5. Day, R. A. & Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India.
6. Freifelder, D. Physical Biochemistry *2nd Ed.*, W.H. Freeman and Co., N.Y. USA 1982.
7. Cooper, T.G. *The Tools of Biochemistry*, John Wiley and Sons, N.Y. USA. 16 1977.
8. Vogel, A. I. *Vogel's Qualitative Inorganic Analysis 7th Ed.*, Pearson, 2013.
9. Vogel, A. I. Vogel's Quantitative Chemical Analysis *6th Ed.*, Pearson, 2009.
10. Robinson, J.W. *Undergraduate Instrumental Analysis 5th Ed.*, Marcel Dekker, Inc., New York 1995.

SEMESTER-V

PHARMACEUTICAL CHEMISTRY

100 Marks

The relation between human health and plants has almost been as old as the civilization. Even today most of the drugs in the market are either plant products or their derivatives. Further the pharmaceutical industries in India is one of the fastest growing industries. The course on "Pharmaceutical Chemistry" will produce suitable human resource to compliment the requirement of pharmaceutical Industries.

1. Brief introduction to the Indian systems of medicine, Indian medicinal and aromatic plants.
2. Extraction, isolation and analysis of phytopharmaceuticals. Importance of natural products, isolation of cinnamaldehyde from cinnamone using steam distillation method.
3. Good Manufacturing Practices (GMP) concept and requirements in the chemical and pharmaceutical plants.
4. Isolation of *p-N*-acetylaminophenol (paracetamol) from crosine® tablet and its characterization by melting point and TLC.
5. Synthesis of paracetamol (*p-N*-acetylaminophenol), purification by crystallization and comparison of melting point and TLC of the synthesized compound with the compound isolated from Tablet in experiment 4.
6. Chiral drugs: current scenario with the case study of thalidomide. Determination of specific rotation, estimation of optical purity of commercially available anti-inflammatory drug, naproxen and its estimation in tablet by acid base titration.
7. Importance of Multi-component reactions in synthesis. Preparation of dihydropyrimidinone, a pharmacophore by classical and greener Biginelli condensation reaction and comparison of the two methodology.
8. Rancidification. Ways of enhancement of shelf-life of oil and determination of rancidity (free acid) in edible oil (fresh coconut oil, stored coconut oil, repeatedly used ground nut oil).
9. Common food adulterants and qualitative analysis of food adulterants in edible oil, milk, milk product and artificial milk.

Recommended Texts:

1. Agrawal, S.S.; Paridhavi, M.; *Chapter 1-3 & 10-11 in Hearbal Drug Technology,* University Press 2007.
2. Dev, S. *A selection of Prime Ayurvedic Plant Drugs*, Ancient-Modern Concordance Anamaya Publishers, New Delhi 2006.
3. Mayo, D.W.; Pike, R.M.; Trumper, P.K. *Microscale Organic Laboratory with Multistep and Multiscale Synthesis 4th Ed.*, Wiley, Chapter 1, and other relevant chapters.
4. Peng, W.; Chen, Y.; Fan, S.; Zhang, F.; Zhang, G.; Fan, X. *Environ. Sci. Technol.* 2010, 44, 9157-9162.

SEMESTER-VI

GREEN CHEMISTRY

100 Marks

It is important that the chemistry students at all the levels whether they intend to pursue careers in science or not be introduced to green chemistry and recognise the impact it can have on human health and the environment. Students should have knowledge of the twelve principles of Green Chemistry which they can apply to their work place after graduation for a safer, less toxic and healthier environment.

The following should be discussed before the experiments are conducted.

- Green Chemistry
- Tools of Green Chemistry.
- Twelve principles of Green Chemistry with examples

1. Safer starting materials

The vitamin C clock reaction using vitamin C tablets, tincture of iodine, hydrogen peroxide and liquid laundry starch.

- Effect of concentration on clock reaction
- Effect of temperature on clock reaction. (if possible)

2. Using renewable resources

Preparation of bio diesel from vegetable oil

3. Avoiding waste Principle of atom economy.

Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.

Preparation of propene by two methods can be studied

(I) Trimethylpropylamine ion + OH^- $\xrightarrow{heat}$ propene + Trimethylamine + water

(II) 1-propanol $\xrightarrow{H_2SO_4/\ Heat}$ propene + water

The other types of reaction like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.

4. Use of enzymes as catalyst

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide

Alternative Green solvents

5. Diels Alder Reaction in water

Reaction between furan and maleic acid in water and at room temperature rather than in benzene and reflux.

6. Extraction of D-limonene from orange peel using liquid CO_2 prepareed form dry ice.

7. Mechanochemical solvent free synthesis of Azomethines

8. Co crystal controlled solid state synthesis (C^3S^2) of N-organophthalimide using phthalic anhydride and 3-aminobenzoic acid.

Alternative sources of energy

9. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II)

10. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

The following Real world Cases in Green Chemistry should be discussed. (Any four)

1 A green synthesis of Ibuprofen which creates less waste and fewer by products. (atom economy)
2 Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments.
3 Environmentally safe antifoulant
4 CO_2 as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market.
5 Using a catalyst to improve the delignifying (bleaching) activity of hydrogen peroxide.
6 A new generation of environmentally advanced preservative: getting the chromium and arsenic out of pressure treated wood.
7 Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
8 Development of a fully recyclable carpet: cradle to cradle carpeting.

Recommended Texts:

1. Anastas, P.T & Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press (1998).
2. Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
3. Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
4. Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. *Green Chemistry Experiments: A Monograph,* I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore ISBN 978-93-81141-55-7 (2013).
5. Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry,* American Chemical Society (2008).
6. Cann, M. C. & Thomas, P. *Real world cases in Green Chemistry,* American Chemical Society (2008).
7. Pavia, D. L. Lamponan, G. H. & Kriz, G.S. *W B Introduction to organic laboratory techniques- a contemporary approach, S*aunders company Philadelphia (1976).