### S.K.E. Society's G.S.S. COLLEGE BELAGAVI P.G DEPARTMENT OF CHEMISTRY Syllabus for Autonomous Status Syllabus of M.Sc. degree in CHEMISTRY

#### FIRST SEMESTER

#### **CHIT-1.1. INORGANIC CHEMISTRY-I**

#### Teaching: 4 h/ week & Total: 64 h

Credits : 4 (16 hr)

#### UNIT–I

#### **CHEMICAL BONDING**

#### **Ionic Bonding**

Formation, conditions for the formation and properties of ionic compounds, lattice energy, Born-Lande's equation, calculation of lattice energy from Born-Lande's equation (problems should be solved), conclusions from Born-Lande equation, Born-Haber cycle, factors affecting the lattice energy. Covalent character in predominantly ionic bonds, polarizing power, factors governing the degree of polarization, Fajan's rules in predicting the melting and boiling points and solubility of some compounds.

Energetics of solubility of ionic salts in polar solvents, solvation energy, relative effects of ionic radii on lattice energy and ion-solvation energy, relative solubility of ionic compounds (alkali metal halides and silver halides, sulphates, and hydroxides of alkaline earth metals).

**Covalent bonding:** Bent's rule of hybridization, illustration of Bent's rule with respect to CH<sub>3</sub>F, PCl<sub>3</sub>F<sub>2</sub>).

**Molecular orbital theory:** Symmetry and overlap, molecular orbital diagrams of diatomic homo nuclear molecules/ions (up to second period elements), heteronuclear molecules/ions (HCl, LiF, CO, NO. Magnetic properties of the molecules/ions based on the MOT, stability of molecules or ions based on bond order.

Metallic bonding: Characteristics of metallic states, V. B. approach, band theory (MOT).

*Self-study*: Valence bond theory: VSEPR theory (sp,  $sp^2$ ,  $sp^3$ ,  $dsp^2$ ,  $sp^3$ d,  $sp^3$ d<sup>2</sup>).

*Skill component*: Determine the bond energy and calculate the lattice energies and discuss their application.

#### UNIT-II

#### CHEMISTRY OF NON-TRANSITION ELEMENTS-I

**Electron deficient compounds**: Classification and nomenclature of boranes: Synthesis, structure and properties of  $B_2H_6$ ,  $B_3H_9$ ,  $B_4H_{10}$ ,  $B_5H_9$ ,  $B_5H_{11}$  and  $B_6H_{10}$ .Polyhedral skeletal electron pair counting using Wade's rules (*styx* numbers): classification of boron clusters using electron pair count.

**Carboranes:** Classification, Nomenclature, Synthesis and structural aspects of closocarboranes  $(C_2B_{10} H_{12})$ .

**Metalloboranes:** Synthesis and structural aspects of  $[B_{11}H_{11}AlCH_3]^{2-}$ ,  $[Fe(CO)_3B_4H_8]$  and  $[2-CpCoB_4H_8]$ .

**Metallocarboranes**: Synthesis of  $[(C_2B_9H_{11})_2Fe]^2$ ,  $[C_2B_9H_{11}FeCp]^-$  and  $[Co(C_2B_9H_{11})_2]^-$ , Structure and Bonding in  $[Co(C_2B_9H_{11})_2]^-$ 

Borazines: Synthesis, reactivity, structure and bonding.

*Self-study*: Electron deficient compound other than Boran and Lewis acids.

*Skill component*: Demonstration on the handling of redox sensitive and air/moisture sensitive materials.

### UNIT-III (16 hr) COORDINATION CHEMISTRY

**Coordination chemistry**: Coordination numbers (1 to 7) and their geometries, geometrical isomerism in square planar and octahedral complexes, optical isomerism in octahedral complexes.

**Bonding theories:** Spectrochemical series (Irwin-William series), Crystal Field Theory, splitting of d-orbitals in octahedral, tetrahedral, square planar, trigonal bipyramidal and square pyramid geometries, Jahn-Teller distortion in co-ordination compounds.

Limitations of CFT, evidences for metal ligand orbital overlap, Molecular Orbital Theory with sigma bonding applied to octahedral, tetrahedral, and square planar complexes. MO-Theory with  $\pi(pi)$ -bonding applied to octahedral complexes.

*Self-study*: Basics of Coordination Chemistry (Review of VBT, EAN and their limitations), CFSE.

Skill component: Methods to identify cis- & trans- as well as L- & D-isomerism.

#### **UNIT-IV**

#### Pi ( $\pi$ ) ACID METAL COMPLEXES AND ACID-BASE CHEMISTRY

**Metal Carbonyls:** Different binding modes of CO, pi ( $\pi$ ) acidity of CO, back bonding, synergic effect, mononuclear carbonyls, low nuclearity carbonyl clusters and high nuclearity carbonyl clusters, application of 18 electron rule to metal carbonyls.

Structural features of  $[Co_2(CO)_8]$ ,  $[Co_4(CO)_{12}]$  and  $[Fe_3(CO)_{12}]$ .

Preparation and structural aspects of Ni(CO)<sub>4</sub>, Fe(CO)<sub>5</sub> and Co<sub>2</sub>(CO)<sub>8</sub> by direct reaction of metals,  $V(CO)_6$ , and  $Mn_2(CO)_{10}$  by reductive carbonylation.

**Dinitrogen Complexes:** Reason for poor coordinating behavior of  $N_2$  compared to its isoelectronic species, binding modes of  $N_2$ , preparation of Ru and Mo dinitrogen complexes.

Acid-Base Chemistry: Lux-Flood theory, solvent-system definition, Usanovich concept, Hammett acidity function (super acids), HSAB theory.

*Self-study*: Bronsted Lowry & Lewis concepts of Acid Base. *Skill component*: Preparation of one metal nitrogen compound and its characterization.

#### **REFERENCE BOOKS:**

01. Inorganic Chemistry: Principles, structure and reactivity, 1997, J. E. Huheey, Keiter and Keiter.

- 02. Inorganic Chemistry, 3rd edition, C. E. Housecroft and A. G. Sharpe.
- 03. Inorganic Chemistry by Purcel and Kotz.
- 04. Inorganic Chemistry by J. D. Lee.
- 05. Inorganic Chemistry by W. W. Porterfield.
- 06. Concepts and Models of Inorganic chemistry by Douglass, Alexander and Mcdaniel.
- 07. Advanced Inorganic Chemistry by Cotton and Wilkinson.
- 08. Inorganic Chemistry by Miessler and Tarr.
- 09. Fundamental concepts of Inorganic Chemistry by A. K. Das, volume 1 to 7.

#### **CHIPr-1.5: INORGANIC CHEMISTRY PRACTICALS-I**

#### Duration: 4 hr/ week & Total: 64 hr

#### Credits : 2

#### Part A. Ore Analysis:

- 01. Hematite: Iron by volumetric using potassium dichromate.
- 02. Pyrolusite: Determination of manganese dioxide in pyrolusite using permanganate titration
- 03. Estimation of calcium and magnesium carbonates in dolomite using EDTA titration, and gravimetric analysis of insoluble residue.

#### Part B. Alloy Analysis:

- 04. Quantitative analysis of Copper-Nickel in alloy /mixture.
  - i. Copper volumetrically using KIO<sub>3</sub>.
  - ii. Nickel gravimetrically using DMG.

#### Part C.

05. Determination of COD and BOD of polluted water.

#### Scheme of Examination:

- i. Duration of examination: 04 hours
- ii. Experiment: 30 marks
- iii. Viva-Voce : 05 marks
- iv. Journal : 05 marks
- v. Internal assessment: 10 marks

#### Total: 50 marks

#### **CHOT-1.2 ORGANIC CHEMISTRY-I**

#### Teaching: 4 hr/ week & Total: 64 hr

### Credits: 4

#### UNIT-I

#### 16 hr

#### **BASIC CONCEPTS AND REACTION MECHANISM**

**Concept of hybridization**:  $sp^3$ ,  $sp^2$ , sp – with examples.

Electronic effects: Inductive, electronic, resonance and hyperconjugation.

**Reactive Intermediates:** carbocations, carbanions, free radicals, carbenes, nitrenes, and arynestheir formation, stability, structure and reactions.

Organic acid and bases: Effect of substituents with examples

Reaction Mechanism: Determination of reaction mechanism by kinetic and non-kinetic-methods.

**Kinetic Method:** Mechanistic implications from rate laws, the transition state theory, ambiguities in interpreting kinetic data, solvent effect, isotopic effect, solvent isotopic effect, substituent effect, steric effect, linear free energy relationships–Hammett equation and Taft treatment.

**Non-kinetic methods**: Energy profile diagram, identification of products, testing possible intermediates, trapping of intermediates, cross over experiments, isotopic labelling, stereochemical studies, limitations.

*Self-study:* Basic of atom, molecules, hybridization, ionization energy, electron affinity, electronegativity, delocalization, Bohr theory, Aufbau principle, steric effect, rate of reaction, activation energy, isotopes, stereochemistry.

*Skill components:* Free radical- ESR spectra of some of the molecule analyzed. Carbocation-isolated compound list and analysis.

#### UNIT-II

16 hr

### ADDITION AND ELIMINATION REACTIONS

#### **Addition reactions:**

Types of addition reactions, mechanism and stereochemistry of addition, effect of substrates and solvents during addition. Addition to Carbon-Carbon double bond; addition of hydrogen halide (Markonikov's & anti-Markovnikov's rule), bromine and peroxide effect. Addition to carbon-hetero multiple bonds (C=O)-Introduction, structure and reactivity; HCN, bisulphate, Grignard reagent, hydride, amino compounds, alcohols and thiols.

#### **Elimination reactions:**

Introduction, types of elimination- $E_1$ ,  $E_2$ ,  $E_{1CB}$  mechanisms, orientation during elimination reactions-Saytzeff and Hoffmann rules, pyrolytic eliminations, Chugaev, Cope eliminations, Hoffmann degradation and dehalogenation of vicinal di halides. Substitution v/s elimination with suitable example.

*Self-study:* Basics of saturated and unsaturated compounds, electrophiles and nucleophiles, geminal and vicinal compounds, difference between addition and elimination reactions. *Skill components:* Analyse some addition and elimination product by FT-IR, UV-vis available from open access/recorded.

#### UNIT-III

16 hr

#### SUBSTITUTION REACTIONS

#### Aromatic electrophilic substitution reactions:

General mechanism of electrophilic substitution in aromatic systems using examples of nitration, halogenations, sulphonation and Friedel Craft alkylation and acylation. Orientation effect of di substitution in aromatic systems with suitable examples.

#### Nucleophilic substitution at saturated carbon:

Mechanism of SN<sub>1</sub>, SN<sub>2</sub>, SN<sub>i</sub> reactions–effect of solvent, substrate and leaving group, neighboring group participation, substitution at vinylic and allylic carbon.

#### Aromatic nucleophilic substitution reactions:

Substitution of hydrogen, substitution other than hydrogen, SN<sub>Ar</sub> reactions, SN1, SN2 and benzyne mechanism, Bucherer reaction.

*Self-study:* Basics of Aromaticity, electrophiles and nucleophiles, electron withdrawing and electron releasing groups and their examples, difference between solute and solvents, vinylic and allylic groups, acids and bases, saturated and unsaturated carbons. stereochemistry (retention & inversion), rate of reaction and activation energy.

*Skill components:* SN<sub>1</sub>, & SN<sub>2</sub> products may be analyzed by polarimeter method and record and analyzed nitration and halogenation products using UV-Vis and FT -IR.

#### **UNIT-IV**

#### **STEREOCHEMISTRY & CONFORMATIONAL ANALYSIS**

**Optical isomerism:** Concepts of chirality-symmetry elements and cause for optical activity, chiral structures, relative configuration- Fischer's DL notation, threo and erythro nomenclature, absolute configurations- R, S nomenclature.

**Molecular presentation:** Sawhorse, Newman, Fischer and fly wedge formulae, enantiomers, epimers, anomers, racemic mixtures, resolution of racemic mixtures-Mechanical, biochemical and chemical method.

**Geometrical isomerism:** Cis-trans, E-Z and syn-anti notations for geometrical isomers, geometrical isomerism in substituted alkenes, oximes, monocyclic and fused and bridge ring system, determination of configuration of geometrical isomers-physical and chemical methods.

**Conformational analysis:** Conformational study of acyclic system (n-butane, ethylene, glycol, chlorohydrin) and cyclic systems cyclohexane chair and boat forms, monosubstituted and disubstituted (1,2, 1,3, 1,4), cis and trans decalins, chirality of cyclohexanes. stereoisomerism in biphenyls, allenes, and spirans

*Self-study:* Basics of stereochemistry, classification, Isomerism, optical activity, chiral compounds, priority order, cis-trans, dextro-levo, oxidizing and reducing agents, plane of polarization.

*Skill components:* Students need to create suitable model for R & S configuration by stick & ball method. Dextro & leavo rotation of some samples record/analyzed by suitable data.

#### **REFERENCE BOOKS:**

01. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ. Press, 1997.

02. Introduction to organic chemistry A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.

03. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1st Edn. Cambridge Univ. Press, 1979.

04. Mechanisms of molecular migrations, Vols I and II, B. S. Thiagarajan, 1st Edn. Pergamon Press, Oxford, 1979.

05. P. J. Garratt in Comprehensive organic chemistry, D. Barton and W. D. Ollis, 1st Edn. Pergamon Press, Oxford, 1979.

06. Radicals in organic synthesis, B. Giese, Pergamon Press, 1986.

07. Stereoelectronic effects in organic chemistry, P. Deslongchamps, 1st Edn. Pergamon Press, 1983.

08. Organic photochemistry, J. M. Coxon and B. Halton, 1st Edn, Cambridge Univ. Press, London, 1974.

09. Molecular reactions and photochemistry, C. H. Deputy and D. S. Chapman, 1st Edn. Prenticehall India, New Delhi, 1972.

10. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley & Sons, 1994.

11. Stereochemistry, Potapov, MIR, Moscow, 1984.

12. Stereochemistry, Nasipuri, D, New Age, 1999.

13. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 2008.

14. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.

15. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2nd Edn. 1998.

16. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2nd Edn., New Age International Publishers, 2001.

17. The text book of stereochemistry, Shikha Agarwal, Dinesh Jangid , Pragati publication, 2019

#### **CHOPr-1.6: ORGANIC CHEMISTRY PRACTICAL-I**

#### Duration: 4 hr/ week & Total: 64 hr

#### Credits : 2

#### **TWO STEP PREPARAT IONS**

- 01. Preparation of acetanilide from aniline
- 02. Preparation of p-bromoacetanilide from acetanilide
- 03. Preparation of hydrolysis of p-bromoacetanilide to p-bromoaniline
- 04. Preparation of p-nitroacetanilide from acetanilide
- 05. Preparation of hydrolysis of p-nitroacetanilide to p-nitroaniline
- 06. Preparation of benzoic acid from benzaldehyde
- 07. Preparation of 2-hydroxynaphthaldehye from 2-naphthol
- 08. Preparation of 2,4,6-tribromo aniline from aniline
- 09. Preparation of phenylazo-β-naphthol
- 10. Preparation of 1-phenyl-3-methyl-pyrazolone

NOTE: Two preparations are to be given for Practical Examinations.

#### Scheme of Examination:

- i. Duration of examination : 04 hours
- ii. Experiment : 30 marks
- iii. Viva-Voce : 05 marks
- iv. Journal: 05 marks
- v. Internal assessment: 10 marks

#### Total: 50 marks

#### **REFERENCE BOOKS:**

01. Vogel's Text Book of Practical Organic Chemistry, Furniss, Hannaford, Smith and Tatchell, ELBS Longmann

02. Advanced Practical Organic Chemistry, N.K. Vishnoi, Vikas, Publishing House

03. Handbook of Practical Organic Chemistry, Clark 04. Practical Organic Chemistry, O.P. Agrawal

#### **CHPT-1.3 PHYSICAL CHEMISTRY-I**

#### Teaching: 4 hr/ week & Total: 64 hr

#### Credits: 4

#### (**16 hr**)

### QUANTUM CHEMISTRY-I

UNIT-I

A brief resume and comparative studies of classical and quantum mechanical phenomenon, Summarization of the results of some experiments (black body radiation, Plank quantum theory, term symbols), Photoelectric and Compton effects. de- Broglie concept (to be derived). Uncertainty principle, Postulates of quantum mechanics, operators, algebra of operators,  $\psi$ properties. Hamiltonian operators and their properties, Schrodinger's equation (with respect to space and time time), derivation for time independent equation, Physical significance and characteristics of wave function, eigen function and eigen values, normalization of  $\psi$ , orthogonality of  $\psi$  boundary valued condition. Particle in one dimension box-derivation of equation Schrodinger's equation with respect to one dimension box (calculation of energy and wave function).

*Self Study*: Basic study about quantum and classical chemistry, study postulates of quantum chemistry, learning linear algebra.

Skill Component: Installation and operating DFT Software.

# UNIT-II (16 hr)

#### **THERMODYNAMICS-I**

Review of basic principles of thermodynamics (I and II laws of thermodynamics, concept of free energy and entropy, combined form of first and second laws of thermodynamics. Entropy change during spontaneous process. Helmholtz and Gibbs free energies. Thermodynamic criteria of equilibrium and spontaneity. Variation of free energy with temperature and pressure. Third law of thermodynamics-calculation of absolute entropies. Thermodynamics of dilute solutions: Raoult's law, Henry's law. Ideal and non-ideal solutions: Liquid-liquid solutions, Azeotropic solutions. Maxwell's relation (to be derived). Thermodynamic equations of equipartition of energy, Clausius clapeyron equation equation (to be derived) and its application. Vant-Hoff's equation, integrated form of van't Hoff's equation. (problems to be solved). *Self Study*: Study terms used in chemical thermodynamics, standard units of measurement of length, weight, time and capacity, zeroth law thermodynamics.

Skill Component: Temperature dependent chemical reactions, explaining state and path functions.

### UNIT–III (16 hr) ELECTROCHEMISTRY –I

Arrhenius theory of strong and weak electrolytes and its limitations, theory of ionic conductance in solutions, ionic atmosphere, relaxation and electrophoretic effects, Debye-Huckel theory of strong electrolytes, Debey-Huckel-Onsagar equation(derivation) and Debey-Huckel limiting law(derivation), quantitative and qualitative treatment of Debye-Huckel limiting law, Onsagar activity co-efficient, mean ionic strength (Debey-Huckel limiting law). A brief survey of Helmholtz-Perrin, Gouy-Chapman and Stern electrical double layer (No Derivation). Fundamentals of batteries, classification of batteries, battery characteristics, primary batteries, dry cell, alkaline MnO<sub>2</sub> batteries and other batteries, secondary batteries-lead acid, lithium batteries, alkaline storage batteries.

*Self Study*: Redox reactions, conductance in electrolytic solutions, specific and molar conductivity, variations of conductivity with concentration, Kohlrausch's law, electrolysis and law of electrolysis (Elementary idea)

Skill Component: Cyclic Voltammetric Study of ferrocyanide/ferricyanide Redox couple.

#### UNIT-IV

(16 hr)

#### POLYMER AND DENDRIMER CHEMISTRY

**Basic concepts**: Monomers, polymers and degree of polymerization, general classification of polymers, homopolymers, copolymers. Polymer molecular weight: Number average and weight average molecular weights. Addition polymers and condensation polymers, comparison between thermoplastics and thermosetting polymers. Transition in Polymers: Definition of glass transition temperature (Tg) and flow temperature (Tf) and melting temperature (Tm). Thermal behavior of amorphous and crystalline polymers, factors affecting Tg. Plasticizers, properties and their effect on Tg. Preparation, properties, and commercial importance: polyethylene, polystyrene, polyvinyl chloride. Ziegler-Natta polymerization, bio-degradable polymers – synthesis and applicationss of poly(ethylene glycol) and poly(vinyl alcohol). Dendrimers and hyper-branched polymers: Introduction to dendrimers, methods of preparation, common properties, and applications.

#### **REFERENCE BOOKS:**

- 01. Physical chemistry Moore, Orient Longman, 1972.
- 02. Principle of polymer science, by Bhahadur and N.V Shastry, 2nd addition Nonasa, 2011
- 03. An introduction to Chemical Thermodynamics –R. P.Rastogi and S.S.Misra, Vikash, Delhi, 1978.
- 04. Thermodynamics -Rajaram and Kunakose, East West, Nagin Cx, Dehli, 1986.
- 05. An introduction to Electrochemistry -Glastone, East west Ltd.
- 06. Electrochemistry principles and applications -Porter
- 07. Introduction to electrochemistry by S. Glasstone.
- 08. Modern electrochemistry Vol. I and II, by J.O.M. Bockris and A.K.N. Reddy, Pentium Press, New York (1970).
- 09. Electrochemistry Principles and applications by E.G. Potter.
- 10. Electrochemistry by Reiger, Prentice Hall (1987).
- 11. Industrial Electrochemistry-D. Pletcher and F.C. Walsh, Chapman, II Edition, 1984
- 12. Introductory Quantum Mechanics Atkins ,Claredon,Oxford
- 13. Quantum chemistry-Kauzman, Academic Press, 1957.
- 14. Quantum chemistry-R.K.Prasad ,II.Ed,New Age Int-2000
- 15. Textbook of polymer science -Billmeyer, Willey Intersection.
- 16. Polymer Science- V. R. Gowariker, 2010.
- 17. Physical Chemistry Gurtu and Gurtu Vol 1 and 2
- 18. Advanced Physical Chemistry Gurdeep Raj
- 19. Physical Chemistry, A Molecular Approach Donald McQuarrie
- 20. Thermodynamics for Chemists Samuel Glasstone
- 21. Quantum Chemistry Ira Levine
- 22. Electrochemistry, Vol 1 and 2 Bockris and Reddy
- 23. Polymer Science Alcock
- 24. Polymer Science Fried
- 25. An Introduction to Macromolecular Science- Aminabhavi and Munk

#### **CHPPr-1.7: PHYSICAL CHEMISTRY PRACTICALS-I**

#### Duration: 4 h/ week & Total: 64 h

#### Credits: 2

#### 1. Conductometry

- a. Acid mixture versus NaOH
- b. Weak acid with salt versus NaOH
- c. Strong acid with salt versus NaOH
- d. To determine the acidic and basic dissociation constant of an amino acid and determination of isoelectric point by pH metry.
- e. Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's law of independent migration of ions.

#### 2. Potentiometry

- 1. K2Cr2O7 versus FAS
- 2. Acid mixture versus NaOH
- 3. KMnO4 versus FAS

4. Determination of dissociation constant of  $H_3PO_4$  using potentiometric method.

5. Determination of pKa value of phosphoric acid by pH meter.

#### **Scheme of Examination:**

- i. Duration of examination: 04 hours
- ii. Experiment: 30 marks
- iii. Viva-Voce: 05 marks
- iv. Journal: 05 marks
- v. Internal assessment: 10 marks

#### Total: 50 marks

#### **REFERENCE BOOKS:**

- 1. Advanced Physico-Chemical Experiments -J. Rose.
- 2. Practical Physical Chemistry -S.R. Palit.
- 3. Experiments in Physical Chemistry Yadav, Geol Publishing House.
- 4. Experiments in Physical Chemistry Palmer.
- 5. Experiments in Chemistry D.V. Jahagirdar, Himalaya Publishing House, Bombay, (1994).
- 6. Experimental Physical Chemistry -Das. R.C. and Behera B, Tata Mc Graw Hill

#### CHAC-1.4 ANALYTICAL CHEMISTRY

#### Teaching: 4 hr/ week & Total: 64 hr

#### Credits: 4

#### UNIT-I

#### (16 hr)

#### DATA ANALYSIS

Classification of analytical methods: Types of instrumental analysis, analytical methods on the basis of simple size. Statistical treatment of finet samples, measure central tendency -mean, medium, range, average deviation, relative average deviation, standard deviation, and variance. Students' confidence interval of the mean. Testing for significance, comparison of two means and two standard deviations. Criteria for rejection of an observation-Q test, control chart, propagation of errors. Least square methods of deriving calibration of plots.

Principles of sampling the sampling step. Methods for sampling solid, liquid and gaseous samples. Effect of sampling uncertainties. Sampling hazards, need for quality assurance: ISO 9000 series of quality of system.

*Self-study*: Errors, types of errors, determinate and indeterminate errors, accuracy and precision. Distribution of random errors, frequency distributions normal error curves. Significant figures. *Skill components*: Students should able to identify the errors occurred during the volumetric (Ore/Alloy) analysis by laboratory method.

### UNIT-II (16 hr) CHROMATOGRAPHY

Introduction, Principles, classifications, fundamentals of chromatography (Partition coefficient, Retardation factor, retention volumes), Dynamics of chromatography

(Efficiency, zone spreading, eddy diffusion) chromatograms, retention time and column efficiency, plate theory and rate theory, Van-Deemeters equation, column resolution, factors influencing resolution.

#### ION EXCHANGE CHROMATOGRAPHY

Introduction, principle, classification of ion exchange resins, mechanism of ion exchange, synthesis of ion exchange resins (cation and anion), characteristics of ion exchange resins (size, capacity, cross linking and swelling and resistance) applications in analytical and metal separations.

#### HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

14

Introduction, principles, instrumentation, mobile phase, stationary phase, types of column, various detectors used, and applications.

*Self-study*: Basics of Chromatography, TLC, R<sub>f</sub> value.

*Skill components*: Prepare the TLC plates, analyze the mixtures, identify and check the purity of compound.

#### UNIT-III (16 hr)

#### SEPERATION TECHNIQUES AND THERMAL METHODS OF ANALYSIS

**Solvent Extraction:** Definition, types, principle and efficiency of extraction, sequence of extraction process, factors affecting extraction-pH, oxidation state, modifiers, synergistic, masking and salting out agents, techniques-batch and continuous extraction, applications, Separation of lanthanides.

**Thermal Methods of Analysis:** Introduction, thermogravimetric analysis (TGA), types of thermogravimetric analysis, principle and method, automatic thermogravimetric analysis, instrumentation, types of recording thermobalances, sample holders, factors influencing thermograms and applications, isothermal analysis, Differential Thermal Analysis (DTA), principle of working, theory and instrumentation, simultaneous DTA-TGA curves, factors affecting results and applications. Differential Scanning Colorimetry (DSC), principle of working, theory, instrumentation, and applications.

*Self-study*: Types of titrations and gravimetric analysis.

*Skill components*: Students should be able to do the binary mixture separation of given compounds by using separation technique (Solvent extraction).

### UNIT-IV (16 hr) ELECTROANALYTICAL TECHNIQUES

Introduction, electrochemical cells, faradic and non-faradic current, mass transfer in cells, galvanic and electrolytic cells, anodes and cathodes, liquid junction potential, schematic representation of cells.

**Polarography**: Theory, principle and applications classical polarography, dropping mercury electrode, polarogram, polarographic measurements, polarographic current, Ilkovic equation, current and concentration relationship, half wave potential, oxygen interference- advantages and limitations. Qualitative and quantitative analysis. Derivative polarography.

Amperometry and Coulometry at controlled potential and at constant current.

**Cyclic voltammetry** - basic principles, instrumentation and applications, stripping voltammetry and its applications including Electro -organic synthesis.

Electrogravimetry - theory, electrode reactions, over-voltage, characteristics of a good deposit, completeness of deposition, Determination of copper and nickel in Cu- Ni alloy.

*Self study*: Basics of electrochemical cells, galvanic and electrolytic cells, polarography, Qualitative and quantitative analysis.

*Skill components*: Students need to do the chemical analysis of the given reducible/oxidizable substances using polarogram.

#### **REFERENCE BOOKS:**

01. Principle of Quantitative Chemical Analysis – Robert de levie, International edition (1997) McGraw Hill Co.

02. Quantitative Analysis- Day and Underwood, Prinitce Hall Indian, Pvt Ltd 6thedition (1993).

03. Vogel's Textbook of quantitative chemical analysis- Revised by G.H.jaffery, J Bassett, J. Mendhm and R.C. Denney ELBS 5thedition (1998).

04. Quantitative Chemical Analysis: D.C Harris W.M. Freeman and Co, NY, USA, Ed, (1995).

05. Introduction to Instrumental Analysis – R.D Brun, McGraw Hill Book company (1982).

06. Physical Methods in Inorganic Chemistry- R. Drago, Affiliated to East west Pvt, (1968).

07. Introduction to chromatography- theory and practice-V.K. Srivastava and K.K.Srivastava, S. chand Company Ltd., IV Ed (1991).

08. Basic Concepts of analytical Chemistry- S.M Khopkar, New Age Intentional Publishers, IIEd.,(1998).

09. Analytical chromatography- G.R Chatwal, Himalaya Publishing House, VII Ed., (1998).

10. Principle Instrumental Analysis- Skoog, Hollar and Nieman, , Harcourt, Asia pvt Ltd., Indian New Delhi, VEd, (1998).

11. Fundamentals of Analytical Chemistry- Skoog, West and Hollar, Harcourt, Asia pvt Ltd., Indian New Delhi, VEd, (1998).

#### CHACPr 1.8:

#### **Analytical Chemistry Practical - I**

#### Duration: 4 hr/ week & Total: 64 hr

Credits: 2

#### I. Organic Chemistry Practical

#### Quantitative analysis

- 1. Titrimetric Estimation of amino acids.
- 2. Estimation of glucose by Bertrand's method.
- 3. Estimation of keto group.
- 4. Iodine value of oil (Chloramine T method)
- 5. Estimation of Nitro group by reduction using SnCl<sub>2</sub>.

#### **Qualitative Analysis**

Separation of binary mixture of organic compounds using ether and identification of separated compounds by systematic qualitative organic analysis.

Please Note:

1) Individual organic compounds are to be given after the candidate reports the nature of the mixture.

2) Ether insoluble acids and ether insoluble Neutral organic compounds may be given.

3) Low boiling liquids and Amino acids need not be given.

The following mixtures may be given.

- 1. Acid + Base
- 2. Acid + Neutral
- 3. Base + Neutral
- 4. Phenol + Acid
- 5. Base + Phenol
- Recrystallization
- Fractional distillation
- Thin layer chromatography
- Column chromatography

### **Scheme of Examination:**

- i. Duration of examination: 04 hours
- ii. Experiment : 30 marks
- iii. Viva-Voce: 05 marks
- iv. Journal: 05 marks
- v. Internal assessment: 10 marks

Total: 50 marks

#### **REFERENCE BOOKS:**

01. Text book of Quantitative Analysis by A. I. Vogel, ELBS, Harlow.

- 02. Advanced Practical Organic Chemistry, N.K. Vishnoi, Vikas, Publishing House
- 03. Handbook of Practical Organic Chemistry, Clark 04. Practical Organic Chemistry, O.P.

Agrawal

#### SECOND SEMESTER

#### CHIT-2.1: INORGANIC CHEMISTRY-II

#### Teaching: 4 h/ week & Total: 64hr

#### Credits: 4

#### UNIT-I

#### (**16 hr**)

#### SYMMETRY AND GROUP THEORY

**Molecular symmetry:** Symmetry elements and symmetry operations, rotation axis, rules for orientation of molecules, plane of symmetry, rotation-reflection axis, centre of symmetry and identity element of symmetry, products of symmetry operations, general relations among symmetry elements and symmetry operations.

**Group theory:** Concept of a group, definition of a point group, procedure for classification of molecules into point groups, subgroups, Schoenflies and Hermann-

Maugin symbols for point groups, multiplication tables for the symmetry operations of simple molecules, matrix notation for the symmetry elements and for geometric transformations, class of a group and similarity transformation.

**Representation of groups:** Reducible and irreducible representations, Great Orthogonality theorem and its consequences, labeling of irreducible representations, group theory and hybrid orbitals to form bonds, character tables (Cs, Ci, C2, C2v and C3v).

**Applications of group theory:** Applications of group theory to crystal field theory, bonding in octahedral and tetrahedral complexes, symmetry and dipole moments, symmetry and optical activity.

*Self-study*: Finding the symmetry elements in compounds with higher CN (> 6)

*Skill component*: Construct the ball and stick model of any chiral compound and deduce the representations.

#### UNIT-II

#### (16 hr)

#### COORDINATION CHEMISTRY-REACTIONS, KINETICS AND MECHANISMS

Types of mechanisms in substitution reactions-dissociation, interchange and association.

Metal-ligand equilibria step-wise and overall stability/formation constant, factors affecting stability of metal complexes. Determination of stability constant by spectrophotometric (Job's) method. Trans/cis effect, thermodynamic and kinetic stability, labile an inert complex, complimentary and non-complimentary reactions.

**Reactions and kinetics of substitution in octahedral complexes:** Ligand field effects and reaction rates, mechanism of substitution in octahedral complexes, reaction rates influenced by acid and base.

**Redox reactions**-outer sphere and inner sphere mechanisms. Marcus theory, excited state outer sphere electron transfer reactions (solar energy conversion).

Photochemistry of metal complexes-type of photochemical reactions, photo substitution and photoredox reaction.

Self study: Fundamental of Solar cell and its reaction mechanism.

Skill component: Find the rate law of substitution reaction using UV-Vis spectrophotometer.

## UNIT –III (16 hr) SOLID STATE AND STRUCTURAL CHEMISTRY

Types of solids, close packing of identical solid spheres, tetrahedral and octahedral voids, packing fraction, and radius ratio.

**Crystallographic systems:** Bravias lattices, Miller indices, external features of crystals. Structures of selected crystals: normal and inverse spinels, hexagonal structures, pervoskites.

**Defects in solids:** Point defects (stoichiometric and non-stoichiometric), line defects and plane defects, stacking faults and grain boundaries.

#### Structural transformation of solids

**Solid solutions:** Hume – Rothery rules, substitutional solid solutions and interstitial solid solutions, solid solution mechanism.

**Alloy systems:** Phase diagram and their features with respect to alloys - two and three component systems, copper–zinc system, steels with reference to iron-carbon systems.

*Self study*: X-ray diffraction technique for powder sample and single crystal. *Skill component*: Indexing of XRD pattern of a cubic system.

### UNIT-IV (16 hr) NUCLEAR CHEMISTRY

Radioactivity, nuclear reactions, nuclear power reactors-radioactivity, determination of half life, radioactive decay kinetics, parent-daughter decay-growth relationships, secular and transient equilibria, nuclear reactions, spallation, nuclear fission and fusion, types of nuclear power reactors,

basic features and components of a nuclear power reactor, safety measures, an introduction to breeder reactors, applications of radioisotopes-synthesis of various useful radioisotopes, physicochemical and analytical applications-isotope dilution method, activation analysis, radiometric titration and 14C dating, medical, agricultural and industrial applications of isotopes.

#### **RADIATION CHEMISTRY**

Interaction of matter with radiation, radiation dosimetry-units and measurement of chemical dosimeters (Fricke and ceric sulphate dosimeters), radiation chemistry of water, a brief introduction to radiolysis of liquids and solids, industrial applications of radiation chemistry (radiation polymerization, food irradiation and radiation synthesis).

**Health and Safety Aspects:** Biological effects of radiation, hazards in radiochemical work, radiation protection, decontamination procedures, permissible exposure doses, nuclear waste management including waste storage and disposal procedures.

Self study: Safety measures from radiation field

**Skill component**: Measuring the radioactivity present in standard sample using GM counter OR construct the Fricke dosimeter and measure the absorbed radiation.

#### **REFERENCE BOOKS:**

01. Symmetry and Spectroscopy of Molecules by K. Veera Reddy.

02. Chemical Applications of Group Theory by F. A. Cotton.

03. Symmetry and Group theory by P. K. Bhattacharya.

04. Inorganic Chemistry: Principles, structure and reactivity, 1997, J. E. Huheey, Keiter and Keiter.

05. Inorganic Chemistry, 3rd edition, C. E. Housecroft and A. G. Sharpe.

06. Inorganic Chemistry by Purcel and Kotz.

07. Inorganic Chemistry by W. W. Porterfield.

08. Concepts and Models of Inorganic chemistry by Douglass, Alexander and Mcdaniel.

09. Inorganic Chemistry by Miessler and Tarr.

10. Introduction to Solids by Azaroff.

11. Solid State Chemistry and its Applications by Anthony R. West.

12. Solid State Chemistry: An Introduction, 3rd edition, Lesley E. Smart and Elaine A. Moore.

13. Fundamental concepts of Inorganic Chemistry by A. K. Das, volume 1 to 7.

14. Essentials of Nuclear Chemistry by H.J. Arnikar, Eastern Wiley (1990).

15. Nuclear Chemistry by U.N. Dash, Sultan Chand and Sons (1991).

#### **CHIPr-2.6: INORGANIC CHEMISTRY PRACTICAL-II**

#### Duration: 4 h/ week & Total: 64 h

#### Credits : 2

#### Part A. Qualitative analysis:

Qualitative analysis of at least FIVE ternary mixtures containing one rare cation and one interfering anion.

#### Part B: Preparation of complexes:

- 1) Copper glycine complex: cis and trans forms
- 2) Optical isomers of  $[Co(en)_3]^{3+}$
- 3) Tris thiourea copper (I) sulphate monohydrate
- 4)  $K_3[Al(C_2O_4)_3] 3H_2O.$
- 5) Tris ethylenediamine Ni(II) chloride
- 6) Estimation of Copper in tristhiourea copper (I) sulphate by Iodometric method.

#### Scheme of Examination:

- i. Duration of examination: 04 hours
- ii. Experiment: 30 marks
- iii. Viva-Voce:05 marks
- iv. Journal :05 marks
- v. Internal assessment: 10 marks

#### Total: 50 marks

#### **CHOT-2.2: ORGANIC CHEMISTRY-II**

#### Teaching: 4 h/ week & Total: 64hr

#### Credits: 4

#### UNIT-I

#### (16 hr)

#### NAMED REACTIONS

**C-C bond forming reactions:** Aldol condensation, Dickmann condensation, Stobbe condensation, Micheal addition, Perkin reaction, Reimer-Tiemann reaction, Reformtsky reaction, Wittig reaction, Mannich reaction, Shapario reaction.

**C-N bond forming reactions:** Chichibabin reaction, Barton reaction, Hofmann-Loffler-Freytag reaction, Stork enamine reaction.

C-O bond forming reactions: Sharpless asymmetric epoxidation, Bayer-Villeger reaction.

C-Cl bond forming reaction: Hell-Volhard-Zelinski reaction.

*Self-study:* Basic of reaction mechanisms, addition, substitution and rearrangement reactions. Stereochemistry.

*Skill components:* Aldol condensation, Michel addition & HVZ reaction products are analyzed by spectroscopic (FT-IR, UV-Vis and NMR spectroscopy) available from online sources.

#### UNIT-II (16 hr)

#### **OXIDATION AND REDUCTION REACTIONS**

#### **Oxidation reactions:**

Introduction, Oxidation reactions examples and applications of chromium series-K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>, PDC, PCC, Sorret and Jones reagents. Manganese compounds-KMnO<sub>4</sub>, MnO<sub>2</sub>.

Oxidation reactions involving ozone, peracids, lead tetra acetate, per iodic acid, osmium tetroxide, selenium dioxide, Oppenauer oxidation.

#### **Reduction reactions:**

Introduction, Catalytic hydrogenation-both heterogeneous (examples Nickel and palladium) and homogeneous, metal hydride reductions (NaBH<sub>4</sub> and LiAlH<sub>4</sub>), reduction with dissolved metal, diimide reduction, Birch, Clemmenson, Wolf Kishner, Meerwin-Varley-Ponndorf reduction, Leukart reaction and reductions with diborane.

*Self-study:* Basics of oxidation and reduction, calculation of oxidation number, oxidizing and reducing agents with examples.

*Skill components:* Oxidizing and reducing agents are identified with model reaction (two examples), and monitor reaction using TLC, UV-Vis and FT-IR.

#### UNIT –III (16 hr)

#### **REARRANGEMENT REACTIONS**

Classification and general mechanistic treatment of nucleophilic, electrophilic, and free radical rearrangements.

**Rearrangement reactions involving migration to electron deficient carbon:** Pinacolpinacolone, Wolf, Wagner-Meerwein, and Benzil-benzilic acid rearrangement.

**Rearrangement reactions involving migration to electron rich carbon:** Favorskii, Sommelet-Hauser, Naber and Steven rearrangement.

**Rearrangement reactions involving migration to electron deficient nitrogen:** Hoffmann, Curtius, Schmidt, Beckmann, Lossen rearrangement.

**Rearrangement reactions involving migration to electron deficient oxygen:** Dakin, Bayer-Villiger and Hydroperoxide rearrangement.

*Self-study*: Basics of rearrangement, nucleophiles, electrophiles and free radicals with examples, migration and rearrangement of atoms, electron rich and electron deficient atoms.

*Skill components*: Students need to give one nucleophilic, electrophilic & free radical rearrangement reactions with suitable examples, analyze reactants and products using spectral data (record/online source).

#### UNIT-IV

(16 hr)

### **Heterocyclic Compounds**

Nomenclature, structure, reactivity, synthesis and reactions of pyrazole, isoxazole, isothiazole, imidazole, oxazole, thiazole.

Indole, benzofuran, quinolone, pyridine, Dimroth rearrangement.

*Self-study:* Basics of heterocyclic compounds, nomenclature and examples, aromatic, non-aromatic and anti-aromatic compounds.

*Skill components:* List out each heterocyclic ring contain drug molecule (one each) and give its biological applications with mechanism/mode of action.

#### **REFERENCE BOOKS:**

- 01. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ. Press, 1997.
- 02. Introduction to organic chemistry A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
- 03. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1st Edn. Cambridge Univ. Press, 1979.
- 04. Mechanisms of molecular migrations, Vols I and II, B. S. Thiagarajan, 1st Edn. Pergamon Press, Oxford, 1979.
- 05. P. J. Garratt in Comprehensive organic chemistry, D. Barton and W. D. Ollis, 1st Edn. Pergamon Press, Oxford, 1979.
- 06. Radicals in organic synthesis, B. Giese, Pergamon Press, 1986.
- 07. Stereoelectronic effects in organic chemistry, P. Deslongchamps, 1st Edn. Pergamon Press, 1983.
- 08. Organic photochemistry, J. M. Coxon and B. Halton, 1st Edn, Cambridge Univ. Press, London, 1974.
- 09. Molecular reactions and photochemistry, C. H. Deputy and D. S. Chapman, 1st Edn. Prenticehall India, New Delhi, 1972.
- 10. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley & Sons, 1994.
- 11. Stereochemistry, Potapov, MIR, Moscow, 1984.
- 12. Stereochemistry, Nasipuri, D, New Age, 1999.
- 13. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 2008.
- 14. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.
- 15. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2nd Edn. 1998.
- 16. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2nd Edn., New Age International Publishers, 2001.

#### **CHOPr-2.6 ORGANIC CHEMISTRY PRACTICAL-II**

#### Teaching: 4 h/ week & Total: 64hr

#### Credits: 4

#### ANALYSIS OF BINARY ORGANIC MIXTURE

Systematic qualitative analysis of binary mixture (solid+solid, solid+ liquid). Chemical equations to be discussed for all tests.

#### **Scheme of Examination:**

- i. Duration of examination: 04 hours
- ii. Experiment: 30 marks
- iii. Viva-Voce:05 marks
- iv. Journal :05 marks
- v. Internal assessment: 10 marks

#### Total: 50 marks

#### **REFERENCES**

- 01. Vogel's Text Book of Practical Organic Chemistry Furniss, Hannaford, Smith and Tatchell, ELBS Longmann
- 02. Advanced Practical Organic Chemistry N.K. Vishnoi, Vikas, Publishing House
- 03. Handbook of Practical Organic Chemistry Clark
- 04. Practical Organic Chemistry O.P. Agrawal

#### **CHPT-2.3: PHYSICAL CHEMISTRY-II**

#### Teaching: 4 h/ week & Total: 64 h

#### Credits: 4

### UNIT-I (16 hr) QUANTUM CHEMISTRY-II

Particle in three dimension box-derivation of Schrodinger's wave equation w.r.t three dimension box (calculation of energy and wave function), Rigid rotator and harmonic oscillator ,applications of Schrodinger's equation to hydrogen atom (to be derived), quantum numbers and their significance, Approximate methods in quantum mechanics, variations method, linear and nonlinear variation functions, application to the Helium atom, hydrogen molecule and ion, normal and degenerate states, Perturbation theory- first and second order perturbation theory, Slater's determination terms symbols and spectroscopic states.

*Skill development*: Brief explanation and experimental results on Density Functional Theory (DFT).

*Self-study*: Study history of quantum mechanics, overview of electronic structure of molecules, VBT, MOT and DFT

#### UNIT-II

#### (16 hr)

#### STATISTICAL THERMODYNAMICS-II

Statistical thermodynamics: Introduction to statistical thermodynamics, energy states, unit cells, microscopic state and macroscopic state, phase space, system, assembly and ensemble, use of ensemble, micro canonical ensemble, canonical ensemble, probability, thermodynamic probability, molecular basis of residual entropy.

Sterling's approximation, Maxwell Boltzmann distribution law and its applications. Bose-Einstein statistics, Fermi-direc statistics and their comparisons. Derive the relationship between entropy and thermodynamic probability, partition function, thermodynamic functions in terms of partition function (energy, heat capacity, entropy, Gibb's free energy, enthalpy Helmholtz free energy). (problems to be solved).

*Skill development*: Plotting of radial wave functions using origin software *Self-study*: principles of mechanics and ensembles, fundamental postulates of Statistical thermodynamics and applications.

#### **UNIT-III**

(6hr)

#### CHEMICAL KINETICS

Complex reactions: Kinetics of parallel, consecutive and reversible reactions. Chain reactions: Branched chain reactions, general rate expression. Theories of reaction rates: Collision theory and its limitations, Activated complex theory (postulates -derivation). Energy of activation.

Lindemann theory, Hinshelwood's theory of unimolecular reactions.

Reactions in solution: Ionic reactions - salt effects, effect of dielectric constant (single and double sphere models). Effect of pressure, volume and entropy change on the rates of reactions. Cage effect with an example. Fast reactions- Introduction, study of fast reactions by continuous and stopped flow techniques, relaxation methods (T- jump and P-jump methods), pulse and shock tube methods.

*Skill development*: Kinetics Studies of the Bleaching of Food Dyes *Self-study*: study of rate of reaction (average and instantaneous), factors affecting rate of reaction.

### UNIT-IV (16 hr) PHOTOCHEMISTRY

Electronic transitions in molecules, The Franck-Condon principle, electronically excited molecules - singlet and triplet states. Life times of excited states of atoms and molecules. Quantum yield and its determination.

A review of laws of photochemistry – Grottus-Draper law, Beer-Lambert law, Stark-Einstein law. Photo physical processes – kinetics of unimolecular reactions, experiments in photochemistry, photo properties - fluorescence, phosphorescence (Joblonski diagram), chemiluminescence. State diagrams, Stern-Volmer equation (to be derived), lasers in photochemical kinetic studies, photo electrochemistry, solar energy conversion and storage.

Photochemical processes – types of photochemical reactions – electron transfer, photo dissociation, oxidation and isomerization reactions with examples. Photosensitization. Flash photolysis.

*Skill development*: Degradation of Methylene blue using ZnO or TiO<sub>2</sub> nanosemiconductors. *Self-study*: Mechanistic background of electrochemistry, chemistry of electronically excited states.

#### **REFERENCE BOOKS:**

01. Statistical themodynamics by B.C. Meclelland, Chapman and Hall, London (1973).

02. Text book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2 nd edition, (1974).

03. Thermodynamics - Rajaram and Kunakose, East West, Nagin Cx, Dehli, 1986.

- 04. Introductory Quantum Mechanics Atkins ,Claredon,Oxford
- 05. Quantum chemistry-Kauzman, Academic Press, 1957.
- 06. Quantum chemistry-R.K.Prasad ,II.Ed,New Age Int-2000.
- 07. Physical chemistry-Atkins, ELRS, 1982.
- 08. Physical chemistry Moore, Orient Longman, 1972.
- 09. Quantum Chemistry Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
- 10. Theoretical Chemistry S. Glasstone. East West Press, New Delhi, (1973).
- 11. Quantum Chemistry R.K. Prasad, New Age International Publishers (1996).
- 17. Physical Chemistry Gurtu and Gurtu Vol 1 and 2
- 18. Advanced Physical Chemistry Gurdeep Raj
- 19. Physical Chemistry, A Molecular Approach Donald McQuarrie
- 20. Thermodynamics for Chemists Samuel Glasstone
- 21. Quantum Chemistry Ira Levine
- 22. Chemical Kinetics Keith J. Laidler

#### **CHPPr-2.7 : PHYSICAL CHEMISTRY PRACTICALS-II**

#### Duration: 4 h/ week & Total: 64 h

#### Credits : 2

#### **Chemical Kinetics**

- **a.** Determine the specific reaction rate of potassium persulphate-iodide reactionby initial rate method.
- b. Study of kinetics of autocatalytic reaction between KMnO<sub>4</sub> versus oxalic acid.
- c. Evaluation of Arrehenius parameter for the reaction between K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> versus KI (first order)
- d. Study the kinetics of the iodination of acetone in the presence of acid by initial rate method.
- e. Study the acid catalyzed inversion of cane sugar and find out: (i) the order with respect to sucrose, (ii)the rate constant, (iii)compare kinetically strength of two acids(HCL and H2SO4).

#### pH metery:

- a. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and calculation of dissociation constant of the base by pH metry.
- b. Determination of pH of acetic acid with sodium acetate buffer by pH metry method.
- c. Determination of pH of formic acid with sodium formate buffer by pH metry method.

#### **Colorimetric:**

- a. Determination of dissociation constant of a given indicator by colorimetric method.
- b. Verification of Beers lamberts law by colarimetric method and calculation of molar extinction co-efficient (molar absorption co-efficient)
- c. To construct the calibration curve Fe2+-KCNS and Cu2+-NH3 systems and estimate the amount of respective salt present in a given solution by colorimetrically

#### Scheme of Examination:

- i. Duration of examination: 04 hours
- ii. Experiment: 30 marks
- iii. Viva-Voce:05 marks
- iv. Journal :05 marks
- v. Internal assessment: 10 marks

#### Total: 50 marks

#### **REFERENCE BOOKS:**

01. Selected Experiments in Physical Chemistry – Latham.

- 02. Experiments in Physical Chemistry James and Prichard.
- 03. Experiments in Physical Chemistry Shoemaker.
- 04. Advanced Physico-Chemical Experiments –J. Rose
- 05. Experimental Inorganic/Physical Chemistry- Mounir A. Malati.
- 06. Quantitative Chemical Analysis Daniel C. Harris, (2006) 7th edition.

Teaching: 2 h/ week & Total: 32 h

Credits: 2

#### UNIT–I

16 h

#### **ULTRAVIOLET and VISIBLE SPECTROSOPY**

**UV-visible spectroscopy:** Types of transitions and their theoretical interpretation, Beer's law, Lambert's law, Beer's-Lambert's law, limitations, chromophores, auxochromes, effect of substituents on the position of  $\lambda$  max, prediction of  $\lambda$  max for polyenes,  $\alpha$ ,  $\beta$ -unsaturated aldehydes and ketones (Woodward- Fisher rules), aromatic systems and their derivatives. basic components of instrumentation-single and double beam designs, applications-analysis of binary mixtures, measurement of dissociation constants of acids and bases.

Stereochemical factors in electronic spectroscopy. Quantitative electronic spectroscopy, Fluorescence and phosphorescence. Absorption spectra of charge transfer complexes. Symmetry restrictions on the allowdness of electronic transition,

Optical rotatory dispersion and circular dichroism; definition and nomenclature, cotton effect and stereochemistry, the octant rule.

Self study (SS): Basic of UV Visible spectroscopy, emission and absorption spectroscopy.

*Skill component (SC):* Selected organic compounds may record UV-vis absorption of benzophenone, benzaldehyde and substituted compounds. And student needs to study, how to calculate molar extinction co-efficient ( $\epsilon$ ),  $\lambda$  max and concentration of some of the molecules/proteins.

# UNIT–II 16 h

#### **IR** spectroscopy

Vibration of diatomic molecules, vibrational energy curves for simple harmonic oscillator, effects of anharmonic oscillation, vibration-rotation spectra of carbon monoxide(No derivation), expressions for fundamental and overtone frequencies, vibrations of polyatomic molecules–The number of degrees of freedom of vibration, , modes of vibration (CO<sub>2</sub> and H<sub>2</sub>O), fundamental, overtone, combination, hot bands, Fermi resonance, force constant and its significance, theoretical group frequency, intensity of absorption band and types of absorptions,

identification of functional groups- alkanes, alkenes, aromatics, carboxylic acids, carbonyl compounds (aldehydes and ketones, esters), amides and amines, fingerprint region, vibrational coupling, hydrogen bonding, steric effect and ring strain.

Quantitative infrared analysis, Absorbance, slit width, Path lengths, molar absorptivity, Attenuated total reflectants and multiple internal reflectants. Laser Raman spectroscopy, The Raman effect, comparision of IR and Raman spectra.

Self study: Basic of IR spectroscopy, Quantum theory of IR, Polarity of bond,.

*Skill component:* Selected six organic compounds may record FT-IR and analyzed complete spectrum of stretching and bending.

#### REFERENCES

01. Introduction to Spectroscopy. Pavia, Lampman and Kriz, 3rd edition, Thomson.

02. Spectroscopy, B. P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 & 2, 1976.

03. Vibration Spectroscopy Theory and Applications, D. N. Satyanarayana, New age International, New Delhi.

04. Organic Spectroscopy, William Kemp, 3rd edition, Palgrava, 1991.

05. Optical Method of Analysis, E. D. Olsen, McGraw Hill Inc, 1975.

06. Spectroscopy of organic compounds – P. S. Kalasi, Wiley Eastern Ltd, India 1993.

07. Introduction to instrumental analysis – R. D. Braun, McGraw Hill Book company 1982.

08. Physical methods in inorganic chemistry – R. Drago, East West Pvt. Ltd, 1968.

09. Instrumental methods of chemical analysis – Gurdeep Chatwal and Anand.

10. Organic Spectroscopy, 2nd edition– Jag Mohan, Narosa Publishing House New Delhi.

11. Spectroscopy by H. Kaur, Pragati prakashan, 2017

#### [OPEN ELECTIVE]

#### **CHEG-2.5: CHEMISTRY FOR EVERY DAY LIFE**

#### Teaching: 4 h/ week & Total: 64 hr

#### Credits : 4

### UNIT-I POLLUTION

16 hr

Air pollution: Air pollutants, prevention and control, greenhouse gases and acid rain, ozone hole and CFC's, photochemical smog and PAN, catalytic converters for mobile sources, Bhopal gas tragedy.

Hydrologic cycle, sources, criteria and standards of water quality-safe drinking water, public health significance and measurement of water quality parameters-(colour, turbidity, total solids, acidity, alkalinity, hardness, sulphate, fluoride, phosphate, nitrite, nitrate, BOD and COD), water purification for drinking and industrial purposes.

Toxic chemicals in the environment.

Detergents- pollution aspects, eutrophication. Pesticides and insecticides- pollution aspects, heavy metal pollution, solid pollutants -treatment and disposal, treatment of industrial liquid wastes. Sewage and industrial effluent treatment.

**Oils and fats:** Composition of edible oils, detection of purity, rancidity of fats and oil, tests for common edible oils Tests for adulterants like argemone oil and mineral oils.

### UNIT-II 16 hr INDUSTRIAL CHEMISTRY

**Composition of soil** - Inorganic and organic components in soil- micro and macro nutrients. **Fertilizers:** Classification of Fertilizers- straight fertilizers, compound/complex fertilizers, fertilizer mixtures, manufacture and general properties of fertilizer products-Urea and DAP. **Ceramics:** general properties, porous and non-porous wares, Manufacturing process, extrusion, turning, drying, decoration, Porcelain and china.

Cement: Types, manufacture, additives, setting, properties & testing of cement.

**Glass:** Manufacture, properties, shaping of sheets & plate glasses. Annealing, finishing. special glasses.

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**Paints and Pigments:** White pigments (white lead, ZnO, lithopone, titanium dioxide), blue, red, yellow and green pigments. paints and distempers, requirements of a good paint, emulsion, latex, luminescent paints, fire retardant paints, varnishes, enamels, lacquers, solvents and thinners.

### UNIT-III 16 hr BIOORGANIC COMPOUNDS

**Carbohydrates:** Chemistry of important derivatives of monosaccharides - ethers, esters, acetals, ketals, deoxysugars and aminosugars.

**Vitamins:** Classification and Nomenclature. Source and deficiency diseases, biological functions of Vitamins- Vitamin A2, Vitamin B, Vitamin C, Vitamin D & Vitamin K. 32

**Food Analysis:** Dairy products- composition of milk and milk products, analysis of fat content, minerals in milk and butter, Estimation of added water in milk.

**Beverages:** Analysis of caffeine in coffee and tea, detection of chicory in coffee, chloral hydrate in toddy, estimation of methyl alcohol in alcoholic beverages.

Food additives, adulterants and contaminants- Food preservatives like benzoates, propionates, sorbates, bisulphites, artificial sweeteners like saccharin, dulcin and sodium cyclamate.

**Flavours:** vanillin, esters (fruit flavours) and monosodium glutamate. Artificial food colourants - coal tar dyes and non-permitted colours and metallic salts. Pesticide residues in food.

**Drugs:** Classification and nomenclature. Analgesics - aspirin, paracetamol; Anthelmentics – mebendazole, Antiallergics - chloropheneramine malleate.

Antibiotics: Pencillin, chloromycetin and streptomycin.

### UNIT-IV 16 hr INDUSTRIAL ORGANIC CHEMISTRY

Chemical energy systems and limitations, principles and applications of primary and secondary batteries and fuel cells, Basics of solar energy, Energy storage devices, Polymers in everyday life: from buckets to rockets: types and classification of polymers, source and general characteristics of natural and synthetic polymers, typical examples of polymers used as commodity plastics, textiles, electronic and automobile components, medical and aerospace materials, problems of plastic waste management, strategies for development of environmental friendly polymers.

**Dyes:** Colour and constitution (electronic concept). Classification of dyes, methods of applying dyes to the fabrics. A general study of Azo dyes, Orange –II, Mordant brown, Congo red and methyl orange.

Corrosion: Types and prevention, corrosion failure and analysis.

#### **REFERENCE BOOKS:**

01. B.K. Sharma: introduction to Industrial Chemistry, Goel Publishing, Meerut(1998).

- 02. Medicinal Chemistry by Asthoush Kar.
- 03. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol.II, INC, New York.
- 04. Analysis of Foods H.E. Cox; 13. Chemical Analysis of Foods- H.E. Cox and Pearson.

05. Foods – Facts and Principles. N. Shakuntala Many and S. Swamy, 4th ed. New Age Internatl (1998).

06. Physical Chemistry - P. Atkins and J. de Paula -7 th Ed. 2002, Oxford University Press

07. Handbook on Fertilizer Technology by Swaminathan and Goswamy, 6 th ed. 2001, FAI.

08. Organic Chemistry by I. L. Finar, Vol. 1 & 2

09. Polymer Science and Technology, J. R. Fried (Prentice Hall)