## A.VEERIYA VANDAYAR MEMORIAL SRI PUSHPAM COLLEGE (AUTONOMOUS), POONDI, THANJAVUR DIST.

## Question Pattern for UG and PG Programmes for students to be admitted during 2014 – 2015 and afterwards

Total Marks: 75

## **QUESTIONS PATTERN**

SECTION – A (Question 1 to 10)

10 x 2 = 20 Marks

- 1. Short Answer Questions
- 2. Two Questions from each units (All are answerable)

## SECTION – B (Question 11 to 15)

5 x 5 = 25 Marks

- 1. 5 Paragraph type questions with "either / or" type choice.
- 2. One question from each unit of the Syllabus.
- 3. Answer all the questions.

#### SECTION – C (Question 16 to 20)

3 x 10 = 30 Marks

- 1. 5 Essay type questions any three are answerable.
- 2. One questions from each unit of the Syllabus.

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
I	14P1CHC1	PHYSICAL CHEMISTRY – I	7	6

#### **UNIT – I Group theory**

**Principles** – Elements of group theory –properties of a group and subgroupclasses- group multiplication tables – symmetry elements and operations – inter relations among symmetry operation point groups of molecules - Matrix representations theory– reducible and irreducible representations – Great orthogonality theorem and its consequences –construction of character tables ( $C_2V$ ,  $C_3V$  and  $C_2h$ )

**Applications of group theory:-** Evaluation of energies and MO's for system like ethylene, butadiene and benzene- hybridization concepts-  $CH_4$  and  $BF_3$  only. Finding symmetry of normal and active modes of vibration for  $H_2O$  and  $BF_3$  only. Symmetry selection rules for IR and Raman Spectra.

#### UNIT – II

#### **Quantum Chemistry – I**

Inadequacy of classical mechanics, Black body radiation, Planck's quantum concepts, Photoelectric effect. Bohr's theory of hydrogen atom: Hydrogen spectra, wave –particle dualism, Uncertainty principle, Inadequacy of old quantum theory.

Schrodinger wave equation, Deviation of time dependent Schrodinger -Postulates of quantum mechanics, **Operator algebra:** operator, linear and hermitian, Verification of operators- Hamiltonian - Eigen functions and Eigen values, angular momentum operator, communication relations, related theorems.

Applications of wave mechanics to simple systems – particle in box, one and three – dimensional, distortion of the box and John –Teller effect, quantum numbers, zero – point energy, orthogonality and normalisation, finite potential barrier – tunneling

#### UNIT – III

**Chemical Kinetics – I** Theories of reaction rates – Absolute reaction rate theory Collision theory – Steric effect – limitations potential energy surface, Transmission coefficient - ARRT theory – thermodynamic treatment – relation with Arrhenius equation Hinshelwood theory, KRR theory – Significance of reaction co- ordinate –Kinetic isotope effect – Marcus theory of electron transfer processes.

Principle of microscopic reversibility – Steady – state approximation - any three examples- specify – Chain reactions. Thermal and photochemical reactions between hydrogen and halogens – Explosions and hydrogen – oxygen reactions.

#### UNIT – IV

**Molecular Thermodynamics** – Calculation of thermodynamic probability of a system – difference between thermodynamic probability and statistical probability – Phase space – Microstate and macro state – methods of determination - derivation of Boltzmann distribution equation – physical significance of partition function – translational, rotational vibrational and electronic partition function.

Relationship between partition function and thermodynamic properties such as E, H, C<sub>P</sub>, C<sub>V</sub>, P. Derivation of PV=RT molecular interpretation of entropy – derivation of S=Klnw Sackur Tetrode equation-Calculation of S, A, G etc from partition functions – calculation of equilibrium constants for very simple reactions.

#### UNIT – V

**Fast reaction Techniques:** Introduction, flow methods (Continuous and stopped flow techniques) – Relaxation methods (T and P jump methods) – Pulse techniques (pulse radiolysis, flash photolysis, Shock tube method) – Molecular beam method.

**Photochemistry:** Basic principles of Photochemistry - Jablonski diagram (Quenching) – Stern – Volmer equation and its applications – experimental techniques in photochemistry -chemical actino meters – laser and their applications.

**Radiation Chemistry:** Differences between radiation chemistry and photochemistry – sources of high energy radiation and interaction with matter – radiolysis of water, solvated electrons – Definition of G value – Curie – Linear energy transfer (LET) and Rad Scavenging techniques – use of dosimeter and dosimeters in radiation chemistry- applications of radiation chemistry.

#### **Reference:**

- 1. Albert Cotton, <u>Chemical Applications of Group Theory</u>, Third Edition John Wiley & Singapore 2003.
- 2. Robert L. Carter, <u>Molecular Symmetry and Group</u> Theory John Wiley and Sons. Inc. New York, 1998.
- 3. R.L. Flurry, Jr. <u>Symmetry Groups</u> Prentice Hall, New Jersy 1980.
- 4. B.E.Douglas and C.A.Hollingsworth, <u>Symmetry in Bonding and Spectra An</u> <u>Introduction</u> Academic Press New York, 1985.
- 5. R.K.Prasad, Quantum chemistry
- 6. A.K. Chandra, Introduction Quantum Chemistry 4<sup>th</sup> ed., Tata McGraw Hill 1984.
- 7. Doggett & Sutelife, <u>Mathematics for Chemists</u>, Longman Scientific & Technical New York, USA, 1995.
- 8. D.A. Mcquarroe, <u>Quantum Chemistry</u>, University Science Books, 1998. F.L. Pillar <u>Elementary Quantum Chemistry</u>, McGraw Hill, 1968.

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
I	14P1CHC2	INORGANIC CHEMISTRY - I	6	5

#### UNIT – I

Acids and Bases: Bronsted and Lewis acids and bases pH, pKa, acid – base concept in non aqueous medium buffer solution , Protonic Acids – Proton Affinities – Differentiating and leveling solvents – Acidic-Behaviour of the Binary hydrides – strength of oxyacids – Hydrolysis – Amphoteric oxides – Non protonic concepts of acid – Base Reactions – Lux concept –Solvent ion theory of Acids and Bases – Liquid Ammonia, Acetic acid, bromine trifluoride, Dinitrogen tetroxide, liquid hydrogen fluoride as solvents – classification on Acids and Bases as Hard or Soft – Acid-Base strength and Hardness and softness –Theoretical basis of Hardness and softness – Electro negativity and Hardness and Softness.

## UNIT – II

**Nuclear Chemistry:** Radioactive decay - Theories of decay processes – Laws of radioactivity – Detection and Measurements of radiations – Nuclear structure – Composition of nuclei – properties of nuclei – nuclear radii – nuclear spin etc. nuclear stability – nuclear models – liquid drop, shell and collective models – Nuclear forces – meson field theory.

**Artificial Radioactivity:** Nuclear reactions – transmutation – Stripping and pick up, Fission products and fission yields, fusion, spallation and fragmentation reactions scattering reactions – nuclear cross section–Q–value Nuclear reactors – charged particle accelerators – neutron sources –gamma ray and X – ray sources . Radioactive techniques – tracer technique neutron activation and isotopic dilution analysis, counting techniques such as G.M. ionization and proportional counter. Applications of nuclear science in agriculture and biology. Radiation risks and medical benefits – Natural and manmade isotopes.

## UNIT – III

**Polyacid anions:** Basic building units of vanadate, molybdate, and tungstate ions – apex sharong (structure only) Heteropoly anions – structure only-Rings Phosphazenes – structure – Craig and Paddock model – Dewar model cages of phosphorus – Boron hydrides and carboranes

**Clusters:** Metal cluster – dinuclar – structures of  $\text{Re}_2\text{Cl}_8$ <sup>2-</sup> qualitative M.O. diagrams for dinuclar rhenium and molybdenum complexes to explain the strength of quadrupole bond – Cluster bonding models – Wade and Luhar.

## UNIT -IV

**Solid state chemistry:** Crystal structure – classification of ionic structure –  $Ax_1$ ,  $Ax_2$ ,  $Ax_3$  types – Ax type (Zns, Nacl, CsCl) structure only –  $AX_2$  type (fluorite, rutile, beto crystobalite) structure only – layer structure –  $CdI_2$ , nickel arsenate. schottky and frenkel defects – explanation and calculation of number of defects per cm – metal excess

defect – F-centre and interstitial ions – metal deficiency defects – positive ion absent – extra interstitial negative ions – semi conductions and transistors – rectifiers – photo voltaic cells.

## UNIT – V

**Main Group Chemistry:** Chemistry of boron – borane higher boranes, carboranes, borazines and boron nitrides. Chemistry of silicon – silanes, higher silanes, multiple bonded systems, disilanes, silicon nitrides, siloxanes and silicates. P-N compounds, cyclophosphazenes S.N. compounds – S<sub>4</sub> N<sub>4</sub> (SN). **Ionic Model:** Lattice energy – Born – Lande equation – born haber cycle-radius ratio-fajans rule-Kapustinski equation – High Tc superconductors – Solid state reactions – Types and examples.

## **References:**

- 1. Badie E.Duglas and Danl H. McDaniel Concepts and models in Inorganic Chemistry, Indian Edition, 1970, Oxford and IBH Publishing Co., New Delhi.
- 2. J.D. Lee. A New concise Inorganic Chemistry, 4<sup>th</sup> Edition, ELBS, 1995 (UNIT II)
- 3. G.Friedlander, J.W.Kennedy and J.M. Miller, Nuclear and Radiochemistry (Unit-III)
- 4. Keith F.P Purchell and John C. Kotz, Inorganic Chemistry, Saunders Golden Sunburst series, W.B. Saunders company, Philadelphia.
- 5. Cotton and Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> Edition, John Wiley & sons, New York (Unit IV)
- 6. W.Kain and B. Schwederski, Bioinorganic Chemistry of life, John Wiley and Sons, New York (Unit V)
- James E. Huheey, Ellen A. Keiter and Richard L. Richard L. Keiter, Inorganic Chemistry Principles of structure and Reactivity, 4<sup>th</sup> Edition, Addition –Wesley, New York (Unit– I)
- Shriver and Atkins, Inorganic Chemistry, III Edition Oxford, 1999, India Gopsons Pvt. Ltd., A – 14 Sector Noida.
- 9. Advanced Inorganic Chemistry Gurdeep Raj 23<sup>rd</sup> reversed and enlarged edition Goal Publishing House, Meerut.

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
I	14P1CHC3	ANALYTICAL CHEMISTRY	6	5

## UNIT I

#### Data and Error Analysis:

Various types of Error – Accuracy, precision, significant figures – Frequency distributions, the binomial distribution, the Poisson distribution and normal distribution – Describing data, population and sample, mean, variance, standard deviation, way of quoting uncertainty, **robust estimators**, repeatability and reproducibility of measurements – Hypothesis testing, levels of confidence and significance, test for an outlier, testing variances, means t-Test, Paired t-Test – Analysis of variance (ANOVA) – Correlation and Regression – Curve fitting , Fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals – General polynomial equation fitting , linearizing transformations, exponential function **fit – r and its abuse** – multiple linear regression analysis, elementary aspects.

## UNIT II

#### Chromatography:

Principles of ion exchange, paper, thin layer and column Chromatography techniques – Columns, adsorbents, methods, Rf values, McReynold's constants and their uses – HPTLC, HPLC techniques – Adsorbents, columns, detection methods, estimations, preparative column – GC-MS techniques: methods, principles and uses.

## UNIT III

**Thermo analytical methods:** Principles, instrumentation and applications of Thermogravimetry Analysis (TGA) – Differential Thermal Analysis (DTA) – differences between TGA and DTA - Differential Scanning Calorimetry (DSC). Thermometric titrations

**Photoelectron Spectroscopy** – Principles – Auger electron spectroscopy – Electron Spectra for Chemical Analysis (ESCA).

#### UNIT IV

**Atomic Absorption Spectroscopy:** Principle – difference between AAS & FES, theory – instrumentation – hallow cathode lamp- burners- oxidants – fuels – interference and applications – Flame Emission Spectroscopy – Principles – instrumentation – interference – limitations of FES – factors that influence the intensity of Emitted radiations – applications – Standard addition and internal standard methods.

#### UNIT V

**Voltametry:** Principles – polarography – principles and introduction instruments current voltage- relationship polarographic waves – equation – half wave potential-reversible and irreversible waves- residual current – migration current – polarographic cells- dropping mercury electrode – advantages of DME – aqua salt bridge- saturated calomel electrode – applications- qualitative and quantitative analysis – inorganic and

organic polarography. Tensametry- chloro potentiometry- instrumentation and applications- Cyclic and stripping Voltametry- principles and applications.

## **References:**

- 1. D.B.Hibbert and J.J. Gooding, Data Analysis for chemistry, Oxford University Press, 2006
- 2. J.Topping, Errors of Observation and their treatment, Fourth Edn., Chapman Hall, London, 1984
- 3. R. Stock and C. B. F. Rice, Chromatographic Methods, Chapman and Hall, New York.
- 4. V.K.Srivastava & K.K. Srivastava, Introduction to Chromatography, S. Chand & Co., New Delhi, 2nd ed,1981.
- 5. Willard, Merrit, Dean and Settle, Instrumental methods of Analysis CBS Publishers and Distributors, 6th ed 1986.
- 6. Skoog, D. A., West, D. M., Holler, F. J., Fundamentals of Analytical Chemistry, 7th edition, Harcourt College Publishers, Singapore. (Pages 523 - 665).
- 7. A.Sharma, S.G. Schulman, Introduction to Fluoresceence Spectroscopy, Wiley-Interscience. New York, 1999
- 8. C.N.Banwell and E.M.McCash, Fundamentals of Molecular spectroscopy, 4th ed., Tata McGraw-Hill, New Delhi, 1994.
- 9. Vogel, A. I., Text book of Quantitative Inorganic Analysis, ELBS.
- 10. Daniel C Harris, Quantitative Chemical Analysis, 4th ed., W. H. Freeman and Company, New York, 1995.
- 11. S.C.Gupta, Fundamentals of Statistics,6th ed., Himalaya Publ. House, Delhi, 2006.
- 12. B.K. Sharma, Instrumental methods of Chemical analysis, Himalaya Publ. House, Delhi, 2006.
- 13. Gurdeep Chatwal, Instrumental methods of Chemical analysis.

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
I	14P1CHCP1	PHYSICAL CHEMISTRY PRACTICAL-I (Electrical)	6	3

## ELECTRICAL

#### **1.CONDUCTOMETRIC TITRATIONS** I.acid – base titrations

- i) Strong acid Vs strong base
- ii) Weak acid Vs strong base
- iii) Mixture of acids Vs strong base
- iv) Mixture of bases Vs strong acid

#### II. precipitaion titrations

- i) KI Vs AgNO<sub>3</sub>
- ii) Mixture of halides (KCl + KI) Vs AgNO<sub>3</sub>
- iii) K<sub>2</sub> SO<sub>4</sub> Vs BaCl<sub>2</sub>

**III.** verification of ostwald's dilution law

IV. Verification of Debye Huckel Onsagar equation

V.determination of solubility of sparingly soluble salt.

#### **2. POTENTIOMETER TITRATIONS**

#### I. acid – base titrations

- i) Strong acid Vs strong base
- ii) Weak acid Vs strong base
- iii) Mixture of acids Vs strong base

#### II. precipitation titrations

- i) KI Vs AgNO<sub>3</sub>
- <sub>ii)</sub> Mixture of halides (KCl + KI) Vs AgNO<sub>3</sub>

#### **III** .Rredox titrations

- i) KMnO<sub>4</sub> Vs KI, FAS
- ii) K<sub>2</sub>Cr2O<sub>7</sub> Vs KI, FAS
- IV. Determination of pH of buffer solutions
- V. Determination of activity coefficient
- VI. Determination of dissociation constant of an organic acid
- VII. Determination of Redox potential of Fe<sup>3+</sup> / Fe<sup>2+</sup> system

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credit
I	14P1CHEL1A	Major Elective-I PHARMACEUTICAL CHEMISTRY	5	4

#### UNIT –I

**Definitions**: The nature and source of drugs, pharmacologically active principles in plants. The terms- Drugs, pharmacology, pharmacognosy, pharmacy, Therapeutics, Toxicology, chemotherapy, pharmacopoeia, First aid –Important rules of first aid - Cuts, Abrasions and Bruises, Fractures, bleeding for blood, maintain breathing. Burns and fainting. First aid box -T.B, Asthma, Jaundice, Piles, Leprosy, Typhoid, Malaria, Cholera, Filariasis - causes- symptoms-diagnosis –prevention and treatment. Medicinally important compounds of Aluminum.

#### UNIT – II

**Antibiotics** : Introduction ,classification–based on biological action, chemical structure. **Chloramphenicol**-assay-synthesis-SAR. **Penicillin** – structure, properties assay -SAR. Semisynthetic production – semi synthetic penicillin -examples – **streptomycin** – structure – assay - SAR.

#### UNIT – III

**Analgesic and Antipyretics**: Narcotic analgesic- analgesic action of morphine, derivatives of morphine, SAR of morphine. Synthetic analgesics- pethidine, methodone-synthesis and uses. Narcotic antagonist – non- narcotic analgesis – methyl salicylate, aspirin, paracetmol, phenacetin ,antipyrine, analgin- preparation, properties and uses. Ibuprofen, ketoprofen, naproxen – structure and uses.

## UNIT – IV

**Anaesthetics:** Ideal anaesthetic agent – classification according to mode of action, General Anaesthetics – volatile ether, vinyl ether, Halothane, Trichloro ethylene – structure, advantages and disadvantages, non-volatile – Thiopental sodium – properties structure, advantages and disadvantages , local anaesthetics- requisites, cocaine-structure and advantages antiseptics and disinfectants – distinction between disinfectants and antiseptics, phenol co-efficient. Psychedelic drugs- lysergic acid diethylamide (LSD)- Pharmacological action of LSD- mechanism of action – therapeutic uses – adverse effects. Marijuana – Pharmacological action and therapeutic uses.

#### UNIT – V

**Cancer**- types, causes, spread, treatment-antineoplastic drugs-alklyating agents, antimetabolise, hormones, antibiotics, radioactive isotopes, adrenocorticostereoids. **Diabetes** -types- control of diabetes insulin, oral hypoglycaemic sulphonyl ureas-tolbutamide, chlorpropamide glibenclamide-structure and uses. Biguanides – phenformin and metformin . **AIDS** – Causes – symptoms – prevention and treatment.

#### **References:**

- 1. Jaya shree ghosh A textbook of pharmaceutical chemistry.
- 2. S. Lakshmi pharmaceutical chemistry.
- 3. K. Bhawate Sundari Applied chemistry.

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credit
I	14P1CHEL1B	Major Elective-I POLYMER CHEMISTRY	5	4

## UNIT – I

**Classification and Molecular weight Determination:** Basic concepts of polymer science – molecular forces and chemical bonding in polymers – classification of polymer – addition polymers, condensation. Major mass and size of polymers – Number average and weight average molecular weight – methods of molecular weight determination. Osmometry viscosity, light scattering, sedimentation, Ultra centrifuge; Molecular weight distribution curve

#### UNIT – II

**Synthesis and Kinetics:** Kinetics of polymerization – free radical chain polymerization, cationic polymerization, anionic polymerization, copolymerization, Degree of polymerization, chain length, chain transfer, chain termination, stereo regular polymerization, zeigler Natta catalysts.

#### UNIT – III

**Characteriation:** Crystalline Nature – X-ray diffraction, study of polymers, degree of crystallinity, Differential scanning Calorimetry, Thermogravimetric analysis of polymers. Glass Transition Temperature – factors affecting Glass Transition Temperature, properties associated with Glass Transition Temperature, Crystallinity and Melting point – Relations to structure.

#### UNIT – IV

**Chemical Reaction Cyclization:** Hydrolysis, Acidolysis, Hydrogenation, Addition and substitution reaction cross linking – Vulcanization, graft and Block Copolymers. Type of degradation – Thermal, Mechanical, Oxidative, Hydrolytic and photo degradation.

#### UNIT – V

**Physical Properties and applications of Polymers:** Mechanical – Stress – strain measurements, Electrical – conducting polymer – polyacetylene, polyaniline. Industrially important polymers – Natural and synthetic rubber – polyesters, polytetrafluoroethylene, (TEFLON), Polystyrene, ion-exchange Resins, polyacrylonitrile – carbon fibres, polyvinyl chloride and polyacrylates.

#### **References:**

- 1. V.R. Gowarikar polymer science, wiley Eastern, 1986
- 2. K.J. Saunders, Organic Polymer Chemistry Chapman and Hall, 1976
- 3. Raymound, B.Seymour, Polymer Chemistry-An introduction, Marcel Dekker Inc. NY 1981
- 4. Fred W. Billmeyer Text book of polymer science, john wiley.
- 5. K. Gupta, fundamentals of polymer science and Engineering, Tata, MgGraw Hill.
- 6. Stepak, polymer characterization of processing technology, Academic press, Indian.

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
11	14P2CHC4	PHYSICAL CHEMISTRY - II	7	6

#### UNIT - I

#### Quantum Chemistry – II

Rigid rotator – harmonic oscillator – rotational and vibrational quantum numbers and selection rules for rotational and vibrational transitions – Bohr's correspondence principle – hydrogen atom – shapes and nodal properties of orbital. Principles of approximation methods – many electron atoms – wave functions – one electron orbital – Pauli's principles and / Slater determinants – variation methods application to hydrogen and helium atoms – perturbation method for non degenerate systems – application of perturbation theory to helium atom. Hartree – Folk self consistent field method – L.S. and J-J coupling. Born – Oppenheimer approximation Huckel pi–election theory and its application to ethylene, butadiene and benzene.

#### UNIT – II

#### **Quantum Statistics**

Quantum statistics – Bose Einstein and Fermi – Dirac statistics – Comparison of them with MB. Statistics – application of B.E. statistics of photon gas and super fluidity of liquid helium. Application of F.D. statistics to electron gas and thermionic emission. Heat capacity of solids – Einstein and Debye's treatment – Concepts of negative Kelvin temperature.

#### Third law of Thermodynamics:

Law of Thermodynamics: Need for the third law – Nernst heat theorem and other forms of stating the third law. Thermodynamic quantities as absolute zero – statistical meaning of third law – apparent exception to the third law.

Non – equilibrium Thermodynamics: Thermodynamics of irreversible processes – Onsager reciprocal relations – steady state conditions.

## UNIT – III

#### Ionics

Transport of ions in solution – Debye – Huckel Onsager theory – Debye – Falkenhagen and wein effects – Modification to Debye – Huckel Onsager theory – Activity of ions in solutions – Experimental determinations – Debye – Huckel limiting law. Activity coefficient at higher concentration – Bejrum model. Electrode – electrolyte equilibrium – Nernst equation and its limitations – equilibrium electrode potential – Classification of electrodes, concentration cells, liquid junction potentials – thermodynamic quantities from EMF data. Electrochemical energy – storage systems – primary and secondary batteries – fuel cells.

#### UNIT – IV

#### **Electro Kinetic Phenomena**

Electrical double layer potential –theory of multilayers at electrode – electrolyte interface – double layers capacity – electro kinetic phenomena – Zeta potential electro osmosis and sedimentation potential.

Process at electrodes – The rate of charge transfer – current density – Butler – Volmer equation – Tafel equation.

Principles of electrode position of metals – electrochemical corrosion metal constructions and use of Pourbaix and Evans diagrams and prevention of corrosion – Electrochemical oxidations and reduction.

## UNIT – V

#### Surface Phenomena

Surface Phenomena: Terminology – Differences between adsorption and absorption- classification- Physisorption and chemisorption- solid – liquid interfaces, solid – gas interfaces, – Factors influencing adsorption of gases on solids- Adsorption isotherms- Freundlich's, Langmuir and BET isotherms – surface area determination. Applications of adsorptions-Activated carbon-application in the treatment of polluted water and air- other applications of activated carbon. Some interfacial aspects on Micelles, Reverse micelles, Micro emulsions and membranes.

#### **Solution Kinetics**

Factors influencing reaction rates in solution – application of ARRT to solution kinetics – effect of solvents double sphere and single sphere model and effect of ionic strength – influence of pressure on rates in solution – Enzyme catalysis – mechanism of single substrate reactions – Michaelis – Menton law – influence of pH and Temperature.

#### **Reference:**

1. S. Glasstone, Introduction to Electrochemistry

- 2. Vogel, A Textbook of Quantitative Inorganic analysis, Longman.
- 3. Bockris and Reddy, Electro chemistry
- 4. P.W. Atkins, Physical Chemistry, ELBS 6<sup>th</sup> edition.
- 5. A.K.Chandra, Introduction to Quantum chemistry
- 6. Donald.A.mcquarrie, Quantum chemistry
- 7. R.K.prasad, Quantum chemistry
- 8. Jain & Jain, Engineering Chemistry.

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
11	14P2CHC5	INORGANIC CHEMISTRY - II	6	5

#### UNIT – I

**Co-ordination Chemistry:** Nomenclature of mono and polynuclear complexes – Crystal field theory – shapes of d orbitals in octahedral symmetry –Splitting in tetrahedral symmetry – only weak field splitting – reasons. Tetragonal symmetry – differences between tetrahedral and tetragonal symmetry. CFSE – Strong Field and weak field splitting – Calculation of CFSE for d<sup>1</sup> to d<sup>10</sup> system. Splitting pattern in trigonal, square planar, trigonal bipyramidal, square pyramidal & cubic symmetries. Factors affecting the magnitude of splitting (10 Dq) – spectro chemical series. Jorgensen's principles. Evidences for CFT. Jahn – Teller distortion – Magnetism and color of transition metal ions, LFT, Nephelauxetic effect.

M.O. Theory – Octahedral, tetrahedral and square planar complexes. Pi bonding and M.O. theory – ligands having filled and empty pi bonds – effect on 10 Dq. Evidences for pi bonding from X-ray Crystallography, IR spectroscopy.

#### UNIT – II

#### **Stability of Co-ordination compounds:**

Labile and inert complexes - Detection of complex formation in solution, stability constants, stepwise and overall formation constants – pH metric, polarographic and photometric methods of determining of formation constants. Factors affecting stability – statistical and chelate effects.

#### Kinetics and mechanisms of reactions in solutions:

Ligand displacement reactions – hydrolysis, equation in octahedral and square planar complexes – Trans effect. Electron transfer reactions – Complementary and non-complementary types – inner sphere and outer sphere processes – isomerization and recemization. Reactions of coordinated ligands, Template effect and syntheses of macro cyclic ligands.

#### UNIT – III

**Inorganic Photochemistry** – Electronic transitions in metal complexes –Various photophysical proceses of coordination compounds – Photsubstitution, photo isomerisation, photo oxidation, photo reduction photochemistry of chromium (III) complexes. Adamson's rules – photochemistry of organometallic compounds, metal carbonyl compounds.

**Main group element** -Periodicity--first and second row anomalies-size effect in non metals-diagonal relationship - nitrogen phosphorous analogies and contrasts- $P\pi$  –  $P\pi$  bonding in heavier non metals. The use of d orbitals by nonmetals-theoretical arguments against d orbital participaton in nonmetals-experimental evidence for bonding.

#### UNIT – IV

**Complexes of pi-acceptor ligands** – Carbonyls – 18 electron rule – Isolobal concept – application to structure of carbonyls (simple and polynuclear). Carbonylate anions, carbonyl hydrides. Nitrosyl complexes – bridging and terminal nitrosyls – Bent

and linear dinitrogen complexes -Metallocenes – reactions – Catalysis by organometallic compounds-ferrocene-hapaticity-carbene complexes-fluxional molecule. Hydrogenation and Hydroformylation of olefins – Oxidation of olefins to aldehydes and ketones – polymerization of alkenes cyclo – oligomeristaion of acetylene – Fischer – Tropsch synthesis.

#### UNIT – V

#### **Bio-inorganic Chemistry**

The biological roles of metal ions, calcium biochemistry, oxygen transport and storage, chlorophyll - carbonic anhydrase, carboxypeptidases, Fe-S proteins and non-heme iron cytochromes of the electron transport chain, cytochrome P-450 enzymes, coenzyme B12, nitrogen fixation and photosynthesis. Metal chelation and the activity of the multipurpose drug.

**Anticancer Activity of Platinum Complexes:** Different types of active Ptcomplexes; toxic effects of anticancer Pt-complexes; mechanism of anticancer activity; nonactivity of trans-platin.

#### **Reference:**

- 1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, Inorganic Chemistry 4<sup>th</sup> ed., Addision Wesley (Unit I, II, III, IV)
- 2. A.W. Adamson, Inorganic photochemistry (Unit III)
- 3. Keith F. Purcell and John C.Kotz, Inorganic Chemistry, Saunders Golden Sunburst Series, W.B. Saunders Company, Philadelphia, 1977.
- 4. W. Kain and B. Sehwederski, Bio Inorganic Chemistry; Inorganic Elements in the Chemistry of life, John Wiley & Sons, New York.
- 5. Shriver, Alkins and Longford, Inorganic Chemistry, ELBS, 1994 (Unit II).
- 6. Asim K. Das, Bioinorganic Chemistry, 2008.

Semester	Subject Code	Title of the Paper	Hours of Teaching /Week	No. of Credits
11	14P2CHC6	PHYSICAL METHODS IN CHEMISTRY – I	6	6

#### UNIT I

#### Theoretical principles of Molecular Spectroscopy:

Interaction of electromagnetic radiation with molecular systems. Transition moment integral and Oscillator strength. Microwave spectroscopy – rotational spectra of diatomic molecules, rigid and nonrigid rotors, - Intensity of spectral lines, - Effects of isotopic substitution – Microwave spectra of polyatomic molecules – Linear and symmetric top molecules, Infrared spectra – diatomic and triatomic molecules, simple harmonic and anharmonic oscillators, - diatomic vibrating rotator, rotation-vibration spectrum of carbon monoxide, - Interaction of rotation and vibration (breakdown of Born – Oppenheimer approximation) – Influence of the rotation on the spectrum of polyatomic molecules, linear and symmetric top molecules, parallel and perpendicular vibrations, Influence of nuclear spin.

#### UNIT II

**NMR:** 1H NMR Spectroscopy – Multiplicity – Coupling constant – First order and second order proton, Spin - spin splitting – Dependence of J on dihedral angle – Vicinal and geminal coupling constants – Karplus equation – long range coupling constants, Influence of stereochemical factors on chemical shift of protons. Simplification of complex spectra – Double resonance techniques, shifts reagents. Chemical spin decoupling of rapidly exchangable protons (OH, SH, COOH, NH, NH2), an elementary treatment of NOE phenomenon. 13C NMR Spectroscopy – Basic theory of FT – NMR, Relaxation – Broad band decoupling. Off resonance decoupling and chemical shifts of common functional groups.

#### UNIT III

## UV –Visible and IR spectroscopy:

#### UV-Visible Spectroscopy:

Introduction - Instrumentation, Sampling techniques - Woodward–Fieser and Scott rules for conjucated dienes and polymers, ketones, aldehydes,  $\alpha$ , $\beta$ -unsaturated acids, esters,nitriles, and amides. Differentiation of geometrical isomers and positional isomers – Disubstituted benzene derivatives - Study of steric effect in aromaticity.

**Infrared Spectroscopy**: Introduction - Instrumentation, Sampling techniques, factors influencing group frequencies – Both internal and external – quantitative studies. Hydrogen bonding – (intermolecular and intramolecular).

#### UNIT IV

**Electron spin resonance spectroscopy:** Basic principles – comparison between esr and nmr spectra – hyperfine splitting – factors affecting the magnitude of g values – calculation of unpaired electron density on an atom in a delocalized system – applications to organic free radicals.

**Mass Spectrometry:** Instrumentation – Resolution, EI and CI methods – Base peak, isotopic peaks, metastable peak, parent peak, determination and use of molecular formula, recognition of molecular ion peak – FAB. Fragmentation – General rules – Pattern of fragmentation for various classes of compounds, McLafferty rearrangement, Importance of metastable peaks.

## UNIT V

**X-ray diffraction**: X-ray diffraction by single crystal – Space groups –Systematic absences in X-ray data and identification of lattice types , glide planes and screw axes.X-ray intensities, structure factor and its relation to intensity and electron density , phase problem.

**Electron Diffraction by gases -** Scattering intensity vs Scattering angle, wierl equation, measurement technique.

**Neutron diffraction by crystals** – magnetic scattering, measurement techniques.

Application of IR, UV, NMR and Mass spectroscopy in the structural elucidation of organic compounds (Minimum 15 problems should be worked out).

## **References:**

- 1. C.N. Banwell, Fundamentals of molecular Spectroscopy, 3rd ed., TMH, New Delhi, 1983.
- 2. B.P. Straughan and S.Walker Spectroscopy Vol.3, Chapman Hall London, 1976.
- 3. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1964.
- 4. P.K.Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley New York, 1989.
- 6. P.M. Silverstein, F. X. Wester, Spectroscopic Identification of Organic Compounds, 6th ed., Wiley 1998.
- 7. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994.
- 8. J.R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall, 1965.
- 9. Y.R. Sharma, Elementary Organic Spectroscopy Principles and Chemical applications, S.Chand, 1992.
- 10. P.S.Kalsi, Spectroscopy of Organic Compounds.
- 11. Clegg,W., Crystal structure determination, Oxford University press, New York, 1998.
- 12. Stout,G.H., Jensen , L.H. X-ray structure determination : A practical guide , John wiley & Sons Publication: New York,1989
- 13. Glusker, J.P., Trueblood,K.N. Crystal structure analysis: A primer., Oxford university press, New York, 1972.

## Webpages:

Cambridge Structural Database (CSD)-<u>http://www.ccdc.cam.ac.uk/products/csd/</u> Protein Data Bank (PDB) <u>http://www.rcsb.org/pdb/home/home.do</u>

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
II	14P2CHCP2	PHYSICAL CHEMISTRY PRACTICAL-II (Non – Electrical)	6	3

#### Non – Electricals

- 1. Determination of CST and study of the effect of impurity on CST
- 2. Determination of distribution coefficient and determination of equilibrium Constant for the formation of  $KI_3$
- 3. Determination of the rate constant for Persulphate oxidation both by titrimetry and Colorimetry.
- 4. Comparison of acid strengths by Kinetics.
- 5. Determination of the energy of activation and frequency factor.
- 6. Association factor of benzoic acid between benzene and water
- 7. Determination of molecular weight by Rast macro method
- 8. Phase diagram simple eutectic system
- 9. Phase diagram three component system
- 10. Adsorption of oxalic acid on charcoal.
- 11. Determination of molecular weight by Transition Temperature Method

M.Sc. Chemistry

Semester	Subject code	Title of the paper	Hours of Teaching/ Week	No. of Credits
II	14P2CHEL2A	Major Elective-II PAINT CHEMISTRY	5	4

#### UNIT – I

**Paint ingredients :** – Classification of paints – according to drying mechanism – under coats – Technical terms , Sag, Skin Irreversible gel, shelf life, Pot life, Solids, vehicle – consistency of thixotrophy – Dry film properties – Adhesion – gloss – flexibility – repair and renovation – Pigments – function (opacity, protective and Reinforcing) – classification – properties – optical – particle size and shape – refractive index – Tinting strength – Chemical reactivity – Bleeding characteristic Hiding power – Examples of pigments – zinc oxide – chrome greens – Lithophone selection of pigments – dispersion – color matching.

#### UNIT – II

Classification of solvents – facts and theory – solvent – properties – boiling point and evaporation rate – uses of solvents –toxicity. Paint additives wetting and dispersing agents. Anti setting – anti – sag and bodying agents – Aluminum soaps – hydrogenated castor oil, modified clays – anti skinning agents – examples – anti flood and anti- float additives – factors influencing flooding and floating – Mildew – inhibitors – dispersing agents (anionic) stabilizing agents (Non ionic) Anti foam agents – thickening agents – preservatives – freezer stabilizers.

#### UNIT – III

Lacquers : Cellulose polymers – acrylic polymers – PMM merits and demerits – film former – industrial application – Emulsions – problems associated – making of Emulsion – merits and demerits – House – hold Emulsion suitable film former – solid content (or) Non Volatile Material (NVM) and Minimum Film Forming Temperature (MFFT) – Drying and semi drying oils – drying mechanism of conjugated and non conjugated Oil Paints – Phenolic resin – Alkyd resin – preparation – properties – House hold air drying alkyd resin – formulation of wood primer.

#### UNIT – IV

**Polyester Rein:** amino resin – uses of amino resin – self polymerization – co reaction – alkyd and polyesters –thermosetting alkyd – urea formuldehyae resin and melamine formaldehyde resin . Ployurethane – raw materials – isocyanate (TDI, MDI, HDI) Hazards of isocyanate – classification of polyurethanes urethane oil and urethane alkyd - Mosisture cure urethane – blocked isocyanate system – two component - polyol type polyurethanes.

#### UNIT – V

**Epoxy Resin** - Manufacture and characterization – curing agents –two pack system – solventless finishes – flooring compounds – fiber glass laminates – single pack thermoplastic epoxy system – water dispersible coatings – powder coatings –Paint film defects -popping – blushing - cissing – yellowing – and orange peel effect

#### **References :**

- 1. G.P.A. Turner –Principles of Paint Chemistry and Introduction to paint Technology Oxford & IBH Publishing & Co
- 2. Paint Film Defects by HESS's
- 3. Modern technology of surface coating & Varnishes by SSP
  - Paint, Lacquers, Enamels, Powder coating & Varnishes by SSP consultan.

Semester	Subject code	Title of the paper	Hours of Teaching/ Week	No. of Credits
II	14P2CHEL2B	Major Elective-II CHEMINFORMATICS	5	4

#### Unit I

**Introduction to Cheminformatics:** Introduction to cheminformatics, History and Evolution of cheminformatics, Use of cheminformatics, Prospects of cheminformatics, Molecular Modeling and Structure Elucidation

#### Unit II

**Representation of Molecules and Chemical Reactions:** Nomenclature; Different types of Notations; SMILES coding; Matrix Representations; Structure of Molfiles and Sdfiles; Libraries and toolkits; Different electronic effects; Reaction classification

#### Unit III

**Searching Chemical Structure:** Full structure search; sub structure search; basic ideas; similarity search; Three dimensional search methods; Basics of Computation of Physical and Chemical Data and structure descriptors; Data visualization.

#### Unit IV

**Computer Assisted Virtual screening design**: Structure Based Virtual Screening- Protein Ligand Docking, Scoring Functions for Protein Ligand docking, Practical aspects of structure based Virtual Screening; Prediction of ADMET Properties, 2 D and 3D data searching, Chemical databases, Role of computers in Chemical Research.

#### Unit V

**Application of Cheminformatics in Drug Design:** Quantitative Structure-Property Relations; Descriptor Analysis; Computer Assisted Structure elucidations; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Design of Combinatorial Libraries; LigandBased and Structure Based Drug design

#### Text Book

1. Andrew R. Leach, Valerie J. Gillet, Cluwer , Introduction to Cheminformatics, Academic Publisher, Netherlands, 2003

#### **Reference Books**

- 1. Lisa B. English (Editor), Combinatorial Library Methods and Protocols, Humana Press Inc, Volume:201, 2002
- 2. Frank Jensen, Introduction to Computational Chemistry, Wiley Publisher, Second Edition, 2006

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
111	14P3CHC7	ORGANIC CHEMISTRY – I	6	5

#### UNIT-I

#### Nomenclature, Heterocyclics and Natural Products

**Nomenclature** of alicyclic, bicyclic,tricyclic compounds (Basic skeletal structures only with or without one substituent) and heterocyclics having not more than two hetero atoms such as oxygen, nitrogen and sulphur

**Heterocyclics:** synthesis and reactivity of the following heterocyclics – pyrazoles, oxazole, imadazole, thiazole, pyridazines and pyrazines.(synthesis of simple alkyl and aryl substituted derivatives are also expected)

**Steroids**: Conversion of cholesterol into progesterone and Testosterone. Stereochemistry and structure elucidation of cholesterol (by chemical degradation)

## UNIT – II

#### Aromaticity

Aromatic character: Five - Six, seven-, and eight-membered rings - Other systems with aromatic sextets – Huckel's theory of aromaticity, Concept of homo aromaticity and anti aromaticity, Electron occupancy in MO's and aromaticity - NMR concept of aromaticity and anti aromaticity, systems with 2,4,8,10 electrons and more than 10 electrons, alternant and non-alternant hydrocarbons. Bonding properties of systems. Heteroaromatic molecules. Annulenes, sydnones and fullerenes.

#### UNIT- III

#### Stereochemistry

Optical activity and criteria for chirality – Enantiotopic, diastereotopic and Prochiral centres. Projection formulae and inter conversions. Absolute configuration – sequence rule - molecules with more than one chiral centre and alicyclic compounds, pseudo asymetric center – RS notataion – Atropisomerism – Geometrical isomerism - EZ notations.

Stereo selective and stereo specific reactions – terminology and principle of stereo selectivity - Asymmetric synthesis and its principle –Meervin Pondorf reduction - Cram's rule . Conformations of di- substituted cyclohexanes and decalins

#### **Dynamic Stereochemistry**

Quantitative correlation between conformation and reactivity. Winstein-Eliel equation-curtin-Hammett principle.Conformation, reactivity and mechanism of cyclic systems - esterfication of an alcohol, chromic acid oxidation of cyclohexanol. De amination of 2-amino cyclohexanol. Conformation, reactivity and mechanism of acyclic systems:Addition reactions, elimination reactions(anti, syn and stereo convergent), NGP and molecular rearrangement.

#### UNIT IV

#### **Nucleophilic Substitution**

Aliphatic nucleophillic substitution:  $S_N 1 S_N 2$ ,  $S_N i$  mechanism -effect of substrate, structure, leaving group, attacking nucleophile and solvent - neigbouring group participation-substitution at allylic carbons and reactivity, ambient nucleophiles-alkylation and acylation of amines, von braun reaction-hydrolysis of esters.

Aromatic nucleophillic substitution:  $S_NAr$ ,  $S_N1$  and benzyne Mechanism - effect of substrate structure leaving group, attacking nucleophile and solvent. zeigler alkylation, Chichibabin reaction -reaction involving diazonium ion, cine substitution, Von Richter reaction.

#### UNIT V

#### **Organic Photochemistry**

Organic Photochemistry – Fundamental concepts – Jablonski diagram – Energy transfer, characteristics of photoreactions, photo reduction and photo oxidation, photoreactions of ketones and enones, Norrish Type I and II reactions. Photochemistry of alkenes, dienes and aromatic compounds Photolytic cycloadditions and photolytic rearrangements – Photosensitization - Photoadditions – Barton reaction – Paterno Buchi reaction.

#### References

- 1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms and structure, 5thed. Wiley, 2000
- 2. D. Nasipuri, Stereochemistry of organic compounds-Principles and applications, New Age International, 2<sup>nd</sup> Edition, 2002.
- 3. I.L. Finar, Organic Chemistry, Vol.II, 5th ed., ELBS 1975
- 4. R.K. Bansal, Organic Reaction Mechanisms, Tata McGraw Hill, 1975.
- 5. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th ed., Pearson, 1992
- 6. J.D. Coyle, Organic Photochemistry Wiley, 1985.
- 7. J.M. Coxon, B. Halton, Organic Photochemistry, Camb. Uni. Press, 2<sup>nd</sup> edition, 1987.
- 8. G.R. Chatwal , OrganicPhtochemistry, Himalaya Publications house, 1<sup>st</sup> edition, 1998.
- 9. P.S. Kalsi, Stereochemistry, Wiley eastern limited, New Delhi, 1990
- 10. V.K.Ahluwalia and R.K.Parashar, Organic reaction mechanisms
- 11. S.M.Mukherji and S.P.Singh, Reaction mechanism in organic chemistry.
- 12. Bhupinder Mehta and Manju Mehta "Organic Chemitry", PHI Learning Pvt Ltd, New Delhi 110001.(2012)

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
111	14P3CHC8	PHYSICAL METHODS IN CHEMISTRY - II	7	6

#### UNIT I

#### **Electronic Spectroscopy**

Term symbols of atoms, ions and molecules – Microstates - energy levels for d1 – d9 ions in cubic and square fields – Intensity of bands – group theoretical approach to selection rules - Effect of distortion and spin-orbit coupling on spectra – Sugano Tanabe diagrams. Orgel diagram for d1 – d9 systems. Evaluation of 10Dq and  $\beta$  for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra.

Optical rotatory dispersion and circular dichroism Cotton effect and ORD curves. Axial haloketone rule, octant rule and its applications. Application of ORD to determine absolute configuration of simple monocyclic ketones.

#### UNIT – II

#### Infrared and Raman Spectroscopy

Vibrations in simple molecules ( $H_2O$ ,  $CO_2$ ) and their symmetry notation for molecular vibrations – Group vibrations and the limitations- combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like  $N_2O$ ,  $CIF_3$ ,  $NO_3$ ,  $CIO_4^-$  –effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide – Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment) – Applications of Raman Spectroscopy – Resonance Raman Spectroscopy.

#### UNIT – III NMR Spectroscopy

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (1H, 19F, 31P, 13C) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei (2H, 10B, 11B) on the 1H NMR spectra, Satellite spectra.

Systems with chemical exchange - study of fluxional behavior of molecules – an elementary treatment of second order spectra – examples – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions.

#### UNIT IV EPR spectroscopy

Theory of EPR spectroscopy - Spin densities and McConnell relationship – Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of V(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

#### Magnetic properties:

Types of magnetism – Dia –para – ferro and antiferro magnetism. Magnetic properties of free ions – first order Zeeman effect – Second order Zeeman effect – states KT – states<KT. Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism. Magnetic properties of lanthanides and actinides.-orbital contribution to magnetic moment, range of  $\mu_{eff}$  for various complexes gouys method Spin crossover in coordination compounds.

#### UNIT V

#### **Mossbauer Spectroscopy**

Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – applications to iron and tin compounds.

#### NQR spectroscopy

Characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

#### **REFERENCES:**

- 1. R.S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern Company.
- 2. R.S.Drago, Physical Methods in Chemistry, W.B. Saunders Company, Philadelphia, London.
- 3. F.A. Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 3rd ed., Wiley-Eastern Company New Delhi 1990.
- 4. P.J. Wheatley, The Determination of Molecular Structure, .
- 5. Lewis and Wilkins, Modern Coordination Chemistry,.
- 6. E.A.V.Ebsworth, Structural Methods in Inorganic Chemistry, 3rd ed., ELBS, Great Britain, 1987.

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
111	14P3CHCP3	ORGANIC PRACTICAL – I	6	3

## 1. Qualitative analysis of organic mixture:

- a. Pilot separation
- b. Bulk separation
- c. Analysis
- d. Derivative

## 1. Separation of amino acids using paper chromatography

## 2. Separation of organic compounds using TLC (CIA ) only

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
111	14P3CHCP4	ORGANIC PRACTICAL – II	6	3

## I. Estimations

- 1. Estimation of phenol
- 2. Estimation of aniline
- 3. Estimation of ketone
- 4. Estimation of glucose
- 5. Estimation of Ascorbic acid

## **II.** Two Stage Preparations:

- 1. Preparation of m-nitro benzoic acid from methyl benzoate
- 2. Preparation of p nitro aniline from acetanilide
- 3. Preparation of aspirin from methyl salicylate
- 4. Preparation of p-bromoacetanilide from aniline

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
IV	14P4CHC9	ORGANIC CHEMISTRY – II	7	6

#### **Unit I: Electrophilic substitution**

**Aliphatic electrophilic substitution**: SE1,SE2and SEi mechanism effect of substrate structure, leaving group, attacking electrophilic and solvent. Stork-enamine reaction decarboxylation of aliphatic acids-halogenation of aldehydes and ketones.

**Aromatic electrophilic substitution:** Arenium ion mechanism-evidenceorientation and reactivity-nitration,halogenations,sulphonation, Friedal crafts reactions-Formylation reaction-Gattermann,Gattermann-koach, Reimer-Tieman and Vilsmeyer-Hack reactions.

# UNIT II: Reactive intermediates and methods of determining reaction mechanism

Generation, reactivity, structure and stability of Carbocations, Carbanions, Carbenes Nitrenes and arynes. **Free radicals** – Configurations – Identification by chemical and spectral methods – Free radical halogenation - NBS.

**Mechanism and methods of determination:** Thermodynamic and kinetic control-Hammond postulate-Microscopic reversibility-intermediate versus transition state.

**Kinetics and non-kinetic methods of determining mechanism** - Product analysis, Determination of the presence of intermediates-isolation, detection and trapping-crossover experiments-isotopic labeling, isotopic effects- stereo chemical evidence-kinetic evidence.

#### **UNIT III: Addition and Elimination Reactions**

**Addition reactions:** Addition to carbon-carbon multiple bond-mechanistic and sterochemical aspects of electrophilic, nucleophilic additions-orientation and reactivity-addition reaction of bromine and hydrogen bromide, hydroxylation, hydroboration, epoxidation oxymercuraton, Michael addition. **Addition to carbonyl groups:** Mannich, stobbe, oppenauer oxidation, MPV reduction, Darzen's glycidic ester condensation, wittig reaction.

**Elimination reactions:** E1,E2,E1CB and Ei mechanism - stereochemistry of elimination, Hofmann and Saytzeff rules- competition between elimination and substitution - chugaev reaction-dehydration of alcohols - dehydro halogenations - Hoffman degradation-cope elimination - Breddt's rule with examples.

**Molecular rearrangement:** Mechanism of the followings - Wagner Meerwin, dienone-phenol, Wolf, Lossen, Schmidt, Bayer-Villeger, Stevens and Favorski rearrangements.

**Reagents in organic synthesis:** Complex metal hydrides-LiAlH<sub>4</sub>,NaBH<sub>4</sub>, ,tritertiarybutoxy aluminium hydride, NaCNBH<sub>3</sub> and tri n-butyl tin hydride DIBAL-H. Lithium dimethyl cuprate, lithium di-isopropylamide, DCC, 1,3-dithane,trimethyl silyl iodide, DDQ, SeO2, Phase transfer catalysis, crown ethers.

#### Unit V: Pericyclic Reactions

Concerted reactions-stereochemistry-conservation of orbital symmetry-FMO method-selectiom rules-electrocyclic, cycloaddition and sigmatropic reactions-1,3 and 1,5 hydrogen shift-cope and claisen rearrangement - fluxional molecule. Woodward Hoffmann rule-correlation diagram method- electrocyclic and cycloaddition only.

#### References

- J. March, Advanced Organic Chemistry: Reactions, Mechanisms and structure, 5<sup>th</sup> ed. Wiley, 2000
- 2. Clayden, Greeves,. Warren and Wothers, Organic chemistry, 2<sup>nd</sup> ed. Oxford University press.
- **3.** Francis A. Carey and Richard J. Sundberg, Advanced organic chemistry part A: Structure and Mechanisms. 5<sup>th</sup> ed.springer
- 4. Francis A. Carey and Richard J. Sundberg, Advanced organic chemistry part B. 5<sup>th</sup> ed.springer
- 5. Peter Sykes, A Guide book to Mechanism in organic chemistry, 6<sup>th</sup> edition Longman, 1986
- 6. P.S.Kalsi, Stereochemistry Conformation and mechanism, 5<sup>th</sup> edition New Age international
- 7. V.K.Ahluwalia and R.K.Parashar, Organic reaction mechanisms. 3<sup>rd</sup> edition, Alpha Science Int'l Ltd
- 8. S.M.Mukherji and S.P.Singh, Reaction mechanism in organic chemistry. 3<sup>rd</sup> edition Macmillan India Limited.
- 9. Bhupinder Mehta and Manju Mehta "Organic Chemitry", PHI Learning Pvt Ltd, New Delhi – 110001.(2012)

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
IV	14P4CHCP5	INORGANIC PRACTICAL - I	6	3

Qualitative Analysis of common and less common cations by Semi – micro

technique in mixtures

## **Common Cations :**

Lead Bismuth, Copper, Cadmium, Antimony, Tin, Iron, Aluminum, Chromium, Manganese, Nickel, Cobalt, Zinc, Calcium, Barium, Strontium, Magnesium and Ammonium.

## Less Common Cations :

Tungsten, Thallium, Selenium, Tellurium, Molybdenum, Cerium, Thorium, Zirconium, Berylium, Uranium, Lithium.

## Complexometric titrations using EDTA

Estimation of Zinc Estimation of Magnesium Estimation of Calcium

M.Sc. Chemistry

Semester	Subject code	Title of the paper	Hours of Teaching/ week	No. of Credit
IV	14P4CHCP6	INORGANIC PRACTICAL – II	6	3

## I. ESTIMATIONS OF MIXTURE SOLUTIONS

- 1. Estimation of Copper and Zinc
- 2. Estimation of Iron and Nickel
- 3. Estimation of Copper and Nickel
- 4. Estimation of Calcium and Magnesium

## II. Colorimetric Estimation of Copper, Iron, Chromium and Nickel

## III. Preparation of the following Inorganic Complexes

- 1. Lead tetra acetate
- 2. Bis ( pyridinium hexa chloroplumbate
- 3. Tris ( thiourea ) copper ( II ) sulphate
- 4. Potassium bis ( oxalate ) aluminate ( II )
- 5. Hexathiourea lead ( II ) nitrate
- 6. Potassium bisoxalato diaquo chromate ( III )
- 7. Hemannine cobalt ( III ) chloride.

M.Sc. Chemistry

Semester	Subject code	Title of the paper	Hours of Teaching/ Week	No. of Credits
IV	14P4CHEL3A	Major Elective - III RECENT TRENDS IN CHEMISTRY	6	4

#### Unit – I

**Nano Chemistry** – Introduction – discovery of CNT, preparation of CNT – arc method – laser ablation method – chemical vapour deposition method, properties – thermal, mechanical, optical, electrical and other properties – uses of CNT. Nano sensors – chemical sensors and biosensors and their uses. Uses of nanotechnology in computers solar energy, fuel cells, medicine and metallurgy.

#### Unit - II

**Nano Synthesis** - Preparation of nano materials by micro wave synthesis – solgel method – chemical co-precipitation – hydrothermal and solvothermal methods. Preparation and uses of  $TiO_2$  and ZnO. Fullerene – preparation – properties and uses. Principle and uses of AFM. Implications of nano science and nano technology on society. Nano shells and their applications.

#### Unit – III

**Green Chemistry** – Introduction, Designing of green synthesis – choice of starting materials, reagents, catalysts and solvents. Twelve principles of green chemistry and their explanation with examples.

**Biocatalysts in organic synthesis:** Introduction – oxidoreductasestransferases – hydrolases-lyases-isomerases-ligases. biochemical oxidations and biochemical reductions-applications.

#### Unit – IV

Green reagents – dimethyl carbonate, polymer supported reagents – (eleven reagents). Green catalysts – acid catalysts, oxidation catalysts, basic catalysts, and polymer supported catalysts – polystyrene aluminium chloride, polymeric super acid catalysts, polymer supported photo sensitizers and phase transfer catalysts. Ionic liquids as green solvents – reactions in acidic ionic liquids and neutral ionic liquids, hydrogenation, Diels – Alder reaction, Heck reaction, O-alkylation and N-alkylation, Methylene insertion reactions.

#### Unit – V

Supra Molecular Chemistry – Concepts and Languages of supramolecular Chemistry – Supramolecular Reactivity and Catalysis.

Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules. Catalysis with Cyclophanes. Type Receptors. Supramolecular Metallocatalysis. Cocatalysis: Catalysis of Synthetic reactions. Biomolecular and Abiotic catalysis.

Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimmers, Gelators. Classification and typical reactions- Applications.

#### **References:**

- 1. New Trends in Green Chemistry by V.K.Ahluwalia & M.Kidwai, Anamaya publishes, New Delhi.
- 2. Chemistry for Green Environment by M.M. Srivastava, Rashmi Sanghi, Narosa publishers, New Delhi.
- 3. Nano the Essential by T. Pradeep. Tata Mc Graw Hill Education Private Limited, New Delhi.
- 4. Supramolecular chemistry.
- 5. Environmental chemistry by B.K.Sharma

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
IV	14P4CHEL3B	Major Elective – III APPLIED CHEMISTRY	6	4

#### Unit-I: Dye Chemistry

**Pretreatment**: Sizing, Desizing- acid method, Scouring- kier boiling method, Bleaching – hypochlorite method, Mersirization, fastness properties – washing, rubbing and light fastness

**Dyeing:** Dye fibre bond, % of shade, M:L ratio, % Of exhaustion, equilibrium absorption, effect of electrolyte.

**Reactive dye** - principles of dyeing. **Polyester dyes** - carrier dyeing - mechanism and high temperature dyeing. **Mordant dyes** - principles - specific examples **Acid dyes**-dyeing mechanism - role of electrolyte and dye bath assistants **Vat dyes** - vatting - dyeing - oxidation and after treatment

#### **Unit-II: Paint Chemistry**

Paint – definitions – ingredients and their role – terminology – emulsion, lacquer. Enamel – pot life, shelf life –varnish – thixotropy –classification of paints based on drying mechanism - under coats – Pigments – classification (organic & inorganic) – functions – properties such as hiding power, light fastness, particle size and shape Solvents used for paints – flash point.

**Vehicles:** Oil – drying mechanism, Description of Alkyd, Epoxy, Polymetyl methacrylate, Urea formaldehyde, Melamine formaldehyde, urethane resins. Additives – Anti skinning agents Powder coating, Solvent less finish.

#### **Unit- III Sonochemistry**

#### The use of Ultrasound in Organic synthesis

Introduction – Instrumentation – The physical aspects – Types of Sonochemical reactions Homogeneous reactions-Heterogeneous liquid-liquid reactionssolid-liquid Heterogeneous reactions-Synthetic Application-Esterification-Saponification-Hydrolysis / Solvolysis- Substitutions - Addition reactions-Alkylationshydroalkylation-Coupling Oxidation-Reduction-Hydroboration-Hydrosilation and reactions-Dichlorocarbene-Other Reactions - Bourgveault reaction-Cannizzaro reaction-Strecker synthesis-The Reformatsky reaction-The barbier reaction of carbonyl compounds-Condensations-Carbohydrates-formation of acetals and benzylidene derivatives of alkylaglycopyranosides.

#### Unit – IV

**Bio Organic Chemistry –** Introduction – definition – Branches of Bio chemistry – Scope – Biomerkenes – functions.

**Carbohydrate** – Introduction – Classification, Mutarotation, Pyronose form, furanose form, Glycogen – structure. **Protein** – Introduction – Classification structure. **Vitamins** – Introduction – Source structure – deficient diseases of B<sub>1</sub>, B<sub>6</sub>, B<sub>12</sub>, A, D– Uses classification. **Alkaloids** – Introduction – occurrence classification. **Nucleic Acid** – RNA, DNA – types of RNA – Differences – Structure of DNA.

#### Unit – V

**Medicinal Chemistry** - Mechanism of drug action and Metabolism of Drugs: Mechanism of action – Drug Receptors and Biological responses – Mechanism of different types of drug action – Metabolism of drugs – Chemical pathway of drug metabolism absorption of drugs – Routes of administration - factors affect absorption – Digestion and absorption of protein – Digestion of fat.