HAJEE KARUTHA ROWTHER HOWDIA COLLEGE

(An Autonomous Institution Affiliated to Madurai Kamaraj University, Madurai.)
Re-Accredited with "A" Grade by NAAC (CGPA of 3.26 out of 4.00)
Uthamapalayam - 625 533

DEPARTMENT OF CHEMISTRY

M.Sc., Chemistry

Syllabus

Academic Year 2017 – 2018 onwards

(I, II, III & IV Semesters)

Programme Specific Outcomes

PSO1. Cognize the nature, functions, and concepts of Organic, Inorganic, Physical, Nano, Medicinal, Analytical and Polymer chemistry

PSO2. Develop and Synthesize chemistry experiments to adopt real life situations

PSO3. Demonstrate reading, listening, writing and speaking skills in communicating subject related topics besides commonplace communications

PSO4. Formulate basic level research ideas in different areas of chemistry

M.Sc., Chemistry
Course Scheme, Scheme of Examinations & Syllabus
Effective from the academic year 2017 – 2018 onwards

Eligibility

A candidate who has passed B.Sc., Chemistry as the major subject with physics as one ancillary. The other ancillary subject may be Mathematics or Botany or Zoology is eligible for the **Master of Science – Chemistry Degree.**

Duration of the Course: M.Sc., Chemistry – 2years (4– Semesters)

Medium of instruction: English

For Programme Completion

A Candidate shall complete:

- Part III – Core papers in semesters I, II, III & IV respectively
- Part IV – Elective papers in semesters I, II, III and IV respectively
- Part IV – Non– Major Elective papers in semester III

Scheme of Examinations under Choice Based Credit System

Term End Examination (TEE)	– 75 Marks
Continuous Internal Assessment Examination (CIAE)	– 25 Marks
Total	– 100 Marks

Pattern of Continuous Internal Assessment Examination (CIAE)

Average of Two Internal Tests (each 20 marks)	– 20 Marks
Seminar	– 05 Marks
Total	– 25 Marks

Pattern of Term End Examination

(Max. Marks: 75 / Time: 3 Hours)

External Examination Question Paper Pattern for Part III & IV
(Core, Non– Major Elective & Elective)

Section – A (10 X 1 = 10 Marks)

Answer ALL questions.

- Questions 1 – 10
- Two questions from each Unit
- Multiple choice questions and each question carries four choices

Section – B (5 X 7 = 35 Marks)

Answer ALL questions choosing either A or B.

- Questions 11 – 15
- One question from each Unit
- Descriptive Type

11 A or 11 B
12 A or 12 B
13 A or 13 B
14 A or 14 B
15 A or 15 B

Section – C (3 X 10 = 30 Marks)

Answer any THREE out of five questions.

- Questions 16 – 20
- One question from each Unit
- Descriptive and Analytical Type

Practical Examination

- Internal – 40 marks (Observation note –10 and Model exam–30)
- External – 60 marks
- Total – 100 marks
- Passing minimum is 40%

DETAILS OF COURSE CATEGORY, CODE, CREDITS & TITLE

Year	Sem	Course Code	Title of the Course	Hours	Credit	Internal	External	Total
I	I	17PCHC11	Introduction to organic reactions	5	5	25	75	100
		17PCHC12	Structure and bonding	5	4	25	75	100
		17PCHC13	Thermodynamics, chemical equilibrium and electrochemistry	5	4	25	75	100
		17PCHC1P	Inorganic qualitative, quantitative analyses and Preparations	10	5	40	60	100
		17PCHE11 / 17PCHE12	**Major Elective** Medicinal and pharmaceutical chemistry / Agricultural Chemistry	5	5	25	75	100
I	II	17PCHC21	Stereochemistry and organic reactions	5	4	25	75	100
		17PCHC22	Coordination and organometallic chemistry	5	5	25	75	100
		17PCHC23	Group theory and spectroscopy	5	4	25	75	100
		17PCHC2P	Organic qualitative and quantitative analyses and preparations	10	5	40	60	100
		17PCHE21 / 17PCHE22	**Major Elective** Analytical chemistry / Industrial Chemistry	5	5	25	75	100

II	III	17PCHC31	Organic spectroscopy and natural products	5	4	25	75	100
		17PCHC32	Inorganic spectroscopy and Nanochemistry	5	4	25	75	100
		17PCHC3P	Conductometric and potentiometric titrations and kinetic, adsorption and spectral measurements	10	5	40	60	100
		17PCHE31 / 17PCHE32	**Major Elective** Quantum, Nano and macromolecular chemistry/ Environmental Science	5	5	25	75	100
		17PCHN31	**Non-Major Elective** Applications of chemistry	5	5	25	75	100
II	IV	17PCHC41	Biomolecules, rearrangements and synthetic methods.	5	4	25	75	100
		17PCHC42	Nuclear and analytical chemistry	5	4	25	75	100
		17PCHC43	Chemical kinetics, surface, biophysical and photochemistry	5	4	25	75	100
		17PCHC4P	Project Project- Viva- Voce	10	4	60	40	100
		17PCHE41 / 17PCHE42	**Major Elective** Polymer chemistry / Conducting Polymers	5	5	25	75	100
Total					**90**			**2000**

Introduction to organic reactions

Programme: **M. Sc., Chemistry** Part: **Core – I**

Semester: **I** Hours: *5*

Subject Code: **17PCHC11** Credits: *5*

Course Outcomes

Determine electron displacements and mechanisms of organic reactions.

Unit I: Electron displacement

Inductive and field effects-Bond distances- Bond energies-delocalized bonds-Cross conjugation-rules of Resonance-Resonance energies-Resonance effects - Steric inhibition of resonance-Hyper conjugation-Hydrogen bonding - Crown ether complexes-Effect of Structure on the dissociation constants of acids and bases.

Introduction to reaction mechanism: Reaction Intermediates-Free radicals, carbocations, carbanions, Carbenes, Nitrenes - formation and stability of reaction intermediates-Methods of determination of reaction mechanism – kinetic and thermodynamic control of Chemical reactions. Kinetic and non-kinetic methods for determining organic reaction mechanism – principle of microscopic reversibility-energy profile diagram-Hammond postulate.

Unit II: Aliphatic Nucleophilic substitutions

Nucleophilicity and basicity-$S_N1$and S_N2 Mechanisms-Effect of substrate structure-Effect of the attacking Nucleophiles-Effect of the leaving group - Effect of the reaction medium-ambident nucleophiles-ambident substrate-Neighboring group participation of n, π and σ electrons-S_NI mechanism-Nucleophilic substitution at an Aliphatic trigonal carbon-Nucleophilic substitution at allylic carbon-Nucleophilic substitution at a Vinyl carbon.

Aliphatic electrophilic substitution: Electrophilic substitution at saturated carbon-S_E1 mechanism, S_E2 and S_EI mechanism.

Unit III: Stereochemistry – 1

Symmetry elements and point group classification-concept of chirality, necessary and sufficient condition for chirality- relationship between substrate symmetry and chirality. Projection formulae-Wedge, Fischer, Sawhorse and Newman. Optical isomerism due to centre of chirality.Molecules with one stereogenic center (Chiral centre) and molecules with more than one chiral centre. Properties of enantiomers and diastereoisomers.Erythro and Threo nomenclature. Configuration - determination of configuration. Cahn, Ingold and Prelog system of designation of configuration.

Geometrical Isomerism: E-Z nomenclature-determination of configuration of geometrical isomers using physical and chemical methods- stereoisomerism in monocyclic compounds (upto six membered rings).

Unit IV: Aromatic character

Aromatic character in Benzene, six membered rings, five, seven and eight membered rings- other systems with aromatic sextets-Huckel's rule- Craig's Rule-concept of Homoaromaticity and Antiaromaticity-Systems with 2, 4, 8 and 10

electrons- Alternate and Non-alternate hydrocarbons. Chemistry of Cyclopentadienyl anion - Fulvene, Azulene, tropolone, sydnones, annulenes.
Novel ring systems: Nomenclature of Bicyclic and tricyclic systems-Chemistry of cubane and catenanes.

Unit V: Oxidation and Reduction

Elimination of hydrogen and aromatization reactions – Catalytic dehydrogenation-Mechanism and applications of the following oxidations – reduction reactions:
Oxidation reactions involving CrO_3, SeO_2, OsO_4, Lead Tetra acetate, Periodic acid, NBS,H_2O_2 - Oppenauer oxidation.
Catalytic hydrogenation-reactions involving lithium aluminum hydride, Sodium Borohydride - Birch reduction - Meerwin-pondoff-verley reduction - wolff- kishner reduction.
Reagents in organic synthesis: Gilman's reagents (Lithium dimethyl cuprate), lithium diisoproylamide (LDA), Tri-n-butyl tin hydride, Wood and Prevost hydroxylation, DDQ, Merrifield resin, Phase transfer catalyst, Peterson's synthesis, Baker yeast.

Books Recommended:

1. P. Skyes, Guidebook to Mechanism to in organic chemistry, Orient Longman, 1976.
2. Jerry March, "Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 5th Edition, Wiley (2000).
3. E.S. Gould, Mechanism and structure in Organic chemistry, Henry Halt & Co. Newyork,1959.
4. J. Shorter, Correlation analysis in organic chemistry, Clarendon press, Oxford, 1973
5. R. T. Morrison, R.N. Boyd, Organic chemistry, Prentice-Hall, 6thedn, 2001.
6. I. L. Finar, "Organic Chemistry", Volume-II, 5th Edition (1975).
7. T. H. Lowry and K. S. Richardson, "Mechanism and Theory in Organic Chemistry", 2nd Edition, Harper and Row, 1981.
8. Reinhard Bruckner, Advanced Organic chemistry, Reaction mechanisms, Academic Press, 2002.
9. F. A. Carey and R.J. Sundberg, Advanced Organic chemistry, Part B, 4th Edition. Plenum Publishers, 2001.
10. R.O.C. Norman, Organic synthesis, 3rd Edition, 1993.
11. W. Carruthers, some modern methods of organic synthesis, Cambridge university press, 2nd edition, 1982.
12. Ho. House, Modern synthesis reactions, W.A. Benkjamin, Inc., California 2nd Edition, 1972.
13. P. S. Kalsi, "Stereochemistry", Wiley Eastern Ltd, 1990.
14. P. Ramesh, Basic principles of Organic stereochemistry, Meenu publications, Madurai, 2005.

Structure and Bonding

Programme: M. Sc., Chemistry Part: Core – II

Semester: I Hours: 5

Subject Code: 17PCHC12 Credits: 5

Course Outcomes

Identify the geometry of molecules, properties of various bonds, different types of solids and their electrical conductivity, various structures in certain inorganic compounds and metals.

Unit I: Nature of chemical bonds

Covalent bond: Hybridization - calculation of s and p characters-Bent's rule-M.O. theory; LCAO approximation-application of MOT to heteronuclear diatomic molecules like $BeCl_2$, BeH_2 and H_2O-concept of multicentered bond as applied to electron deficient molecules like diborane and metal alkyls - VSEPR theory - Walsch diagram AB_2, AB_3.

Unit II: Bond properties and ionic bonding

Ionic radii-covalent radii-vander Waals radius-bond length-Bond order-bond energy, bond polarity-partial ionic character of covalent bonds- electronegativity-electron affinity-lattice energy-Bond land equation-Born Haber cycle-Covalent character in Ionic compounds-Different types of electrostatic interactions -Hydrogen Bond.

Unit III: Solid state chemistry

Crystal defects-points, line and plane defects- Colour centers - Non-stoichiometry on physical properties-Electronic structure of solids- Free electron and band theories-Types of solids-Electrical conductivity and superconductivity-High temperature superconductors-Types of semiconductors-Thermo-electric power and Hall effect-Photovoltaic effect-Semiconductors in solar energy conversion.

Unit IV: Inorganic chains - Rings and cages

Silicates: Various silicate structures-structure, property, correlation-silicones.

Poly acids: Classification-isopolyacids like polymolybdate, polyvanadate and polytungstate - their structures – hetero poly acids: 12A, 12B, 9 and 6 heteropolyacids- preparation and structures.

Phosphazenes and its polymers: Phosphonitrile compounds-S_4N_4-Polymeric sulphur nitride (Polythiazyl) – Boranzine.

Cage Compounds: Nomenclature of Boranes and carboranes-Wades rule- STYX number- preparation and structure of B_4H_{10}, $C_2H_{10}H_{12}$, $(B_{12}H_{12})^{2-}$.

Unit V:

Occurrence, isolation, purification, properties and uses of the following metals as well as their important compounds: Be, Ge, Ti, Zr, Th, V, Pu, U and Platinum.

Books Recommended:

1. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 5th Edition, John Wiley&Sons, Singapore, 1998.
2. K.M. Mackay and R. A. Mackay, Introduction to Modern Inorganic chemistry, 4th Edn. Prentice Hall, New Jersy, 1989.
3. James E. Hugheey, Ellen A. Keitler and Richard L. Keitler, Inorganic Chemistry, 4th Edn, Harper COllinsCOllege Publishes, New York, 1993.
4. P. W. Atkins, D. k. Shriver and C. H. Langfood, Inorganic Chemistry, Oxford ELRS, UK, 1990.
5. K.F. Purcell and J.C. Koltz, An introduction to Inorganic Chemistry, W.B. Saunders Company, Philadelphia, 1980.
6. N.B. Hanny, SOlid State chemistry.

Thermodynamics, Chemical Equilibrium and Electrochemistry

Programme: M. Sc., Chemistry Part: Core – III

Semester: I Hours: 5

Subject Code: 17PCHC13 Credits: 4

Course Outcomes

Recognize laws of thermodynamics, statistical thermodynamics, phase rule and electro chemistry.

Unit I: Thermodynamics

Second law of thermodynamics-concept of entropy-Gibb's function-Gibb's Helmholtz equation-Maxwell relations-Thermodynamic equation of state-Thermodynamics of systems of variable composition- Partial molar quantities, partial molar volume- chemical potential, Gibbs-Duhem equation-Experimental determinations of fugacity of real gases and its determination-Third law of thermodynamics - Absolute entropies-Determination of absolute entropies-Exception to third law- Unattainability of absolute Zero.

Unit II: Chemical and phase equilibria

Reaction free energy/Reaction potential-Reaction isotherm and direction of spontaneity - Standard reaction free energy-its calculation from thermo chemical, electrochemical and equilibrium data-Temperature coefficient of reaction free energy and equilibrium constant.

Gibbs phase rule-its thermodynamic derivation - Application of phase rule to three component systems - Formation of one pair, two pairs and three pairs of partially miscible liquids-Systems composed two solids and a liquid.

Unit III: Statistical Thermodynamics

Aims of statistical thermodynamics -definition of state of system - ensembles (micro, macro and grand canonical)-Boltzmann distribution law and its deviation-Boltzmann-Planck equation-Partition functions-Thermodynamic properties from partition functions-partition function and equilibrium constant-Quantum statistics-Fermi-Dirac and Bose- Einstein's statistics-Photon gas and electron gas according to such statistics-Einstein's and Debye's theories of heat capacities of solids - Calculation of residual entropy of H_2 at 0K in terms of ortho-para ratio.

Unit IV: Electrochemistry I

Theory of electrolytic conductance -inter-ionic attraction-ionic atmosphere - thickness of ionic atmosphere-The Debye-Huckel-Onsager conductance equation-its deviation and experimental verification - deviations and modifications -Debye Falkenhagand and Wein effects-mean ionic activity and activity coefficients of strong electrolytes.

The role of electrodes- the electrochemical potential -types of electrodes-the gas/inert metal electrode-ion/insoluble salt/metal electrode-oxidation-reduction electrode-liquid junction potential -Electrochemical cells -kinds of cells-notation-electrochemical cell reactions -EMF of cells -Nernst equation- Application of EMF measurements -determination of equilibrium constant, dissociation constant, solubility product and potentiometric titrations.

Unit V: Electrochemistry II

The electrical double layer and Zeta potential -Perrin, Gouy-Chappman and Stern models- -Electrokinetic phenomena- Over potential -Butler Volmer equation - Tafel equation-Current-potential curves-hydrogen over voltage.

Application ofelectrochemical processess -power generation and storage- Fuel cells-storage batteries and dry cells-Principles of inhibition of corrosion-cyclic voltammetry-Photo electrochemistry and electrochemiluminescence.

Books Recommended:

1. S. Glasston, Thermodynamics for chemists, East-west Press Private Ltd., New Delhi.
2. J. Rajaram and J.C. Kuriakose, Thermodynamics (III Edn.)Shoban LalNagin, Chand & Co.,Ltd., New Delhi (1999)
3. B.R.Puri,L.R.Sharmaand M.S. Pathania, Priciples of PhysicalChemistry (MilleniumEdn.) Vishal Publishing Co., (2003)
4. Gurdeep Raj, Advanced Physical Chemistry (25th Edn.,) Goel Publishing Co., (2001)
5. D. AMcQuarrie and J.D. Simons, Physical Chemistry - A Molecular Approach,viva Books (P)Ltd., New Delhi (1998)
6. P.W. Atkins, Physical Chemistry. VI Edn., ELPS and Oxford University Press (1996)
7. S.H. Maron and J. B. Lando, Fundamentals of Physical Chemistry, MacMillan Publishing Co., New York (1974)
8. D. N. Bajpai, Advanced Physical Chemistry, S. Chand & Company Ltd., Newelhi(1998)
9. A. Findlay, The Phase Rule and its Applications, Campbell and Smith.
10. A. W. Adamson. Physical Chemistry of Surfaces, 5th Edn., John wiley & Sons, New Delhi (1990).
11. D. Attwood and A. T. Florence, Surfactant Systems-Their chemistry, Pharmacy and Biologyl, Chapman and Hall, New York (1983)

Semester I

Inorganic chemistry practical

17PCHC1P	Inorganic qualitative and quantitative analyses and preparations	Hours 10/Credits 5

1. Semi micro qualitative analysis: analysis of mixtures containing one familiar and one less familiar cations from the following:
   W, Pb, Tl, Se, Te, Mo, Cu, Bi, Cd, Ce, Th, Zr, Ti, V, Cr, Mn, Al, U, Ni, Co, Zn, Ca, Ba, Sr, Li and Mg.
2. Estimation of one metal in the presence of another by EDTA (demonstration)
3. In organic preparations; Preparations of atleast 6 (six) in organic complexes.
4. Quantitative analysis: separation and estimation of mixture by volumetric and gravimetric methods.
   Cu & Ni, Cu &Zn, Ca & Ba, Fe & Ni, Fe & Cu.
5. Preparation of one Ni (II) octahedral complex-its UV-visible spectrum-evaluation of 10Dq, B and β (Demonstration only).

Medicinal and Pharmaceutical Chemistry

Programme: **M. Sc., Chemistry** Part: **Elective – I**

Semester: **I** Hours: *5*

Subject Code: **17PCHE11** Credits: *5*

Course Outcomes

Construe the drugs and their interactions with various organs of humans, synthesis of new drugs and their biological activities, therapeutic uses of steroids, alkaloids and antibiotics.

Unit I: Fundamentals of medicinal chemistry

Definitions of Medicinal Chemistry, Pharmacology and Molecular Pharmacology-major process involved in drug action - Pharmacokinetics phase – Quantitative structureActivity relationship (QSAR)-Hansch approach – Concept of bio-isoterism– Receptors and classification of membrane bound receptors-enzyme inhibitors as drugs (illustrated with one example).

Unit II: Medicinally useful antibiotics and steroids

Structural features and mode of action of the following antibiotics –penicillin G, Cephalosporin and their semi synthetic analogs (β-lactum), Streptomycin (aminogylcoside), Terramycin (tetracyclin), Erythorymycin (macrolide) and Chloramphenicol.

Steroids; Oral contraceptives, anabolic steroids, anti -inflammatory steroids.

Unit III: Chemotheraopeutic agents

Antineoplastic agents:

Classification, synthesis e.g., Cyclophosphamide, Ifofamide, Chlorambucil, Busulfan, Decarbazine, Methotrexate, 6-Mercaptopurine.

Anti-tubercular drugs:

Classification, synthesis, e.g., Isoniazid, Pyrazinamine, Ethambutol, ThiacetoazoneandEthionamide.

Antimalarial drugs:

Classification, synthesis, e.g., Chloroquine, Primaguine, Amaodiaquine, Proguanil and Pyrimethamine.

Diuretics:

Classification, Synthesis, e.g., Furesemide, Acetazolamide, Chlorothiazide.

Unit IV: Synthesis and therapeutic action and SAR of certain drugs

Antihypertensive drugs:

Nifedipine, Captopril, Hydralazine, Sodium nitroprusside and Clonidine.

Antihistamines:

H1-Antagonists: Pheniramine, Chlorpheniramine, Diphenylhydramine, Mepyramine, Promethazine, H2-Antogonist: Cimetidine, Ranitidine and Fomotidine.

Unit V:

Anti-inflammatory drugs

Antipyretics & Non-narcotic analgesics; Aspirin, sodium salicylate, Paracetamol, phenylbuttazone, Oxypheylbutazone, Ibuprofen, Mefenamic acid, Dichlofenac sodium.

CNS stimulant Drugs:

Amphetamine, Caffeine, Theobromine, Theophylline, Bemegride, Nikethamide, MethyPhenidate.

CNS Depresent Drugs:

Phenelazine, Isocarboxazide, Imipramine, Nortiptyline, Amitriptyline, Desipramine.

Books Recommended:

1. G.L. Patrick, An introduction to Medicinal chemistry, II Edn. Oxford University Press, 2001.S
2. T. Nagradi, Medicinal Chemistry – A Biochemical Approach, Oxford University Press-2004.
3. J. B. Taylor and P.D. Kennewall, Introductory Medicinal Chemistry, Ellisworth Publishers, 1985.
4. C. Laxmi, Medicinal Chemistry.
5. B. JeyasreeGhosch, Pharmaceutical chemistry
6. Ashutoshkar Medicinal Chemistry.

AGRICULTURAL CHEMISTRY

Programme: **M. Sc., Chemistry** Part: **Elective – II**

Semester: **I** Hours: **5**

Subject Code: **17PCHE12** Credits: **5**

Course Outcomes

To Acquire knowledge about water analysis, soil analysis, Irrigation, Fertilizers, Pesticides and Insecticides, Fungicide and Herbicides.

Unit I: Water source for Agriculture

Water treatment and water analysis - acidity, alkalinity, pH, Biological oxygen demand (BOD). Chemical oxygen demand (COD) and their determinations, Recycling of water, water management.

Unit: II Chemistry of soil, soil classification and soil analysis

Definition, classification and properties of soil, Soil erosion, Soil fertility, Soil organic matter and their influence on soil properties, Soil reactions- soil pH, acidity, alkalinity, buffering of soils and its effect on the availability of N, P, R. Ca and Mg.

Unit: III Irrigation

Crop Seasons-seed, seed development organization, natural seeds projects phase-III, new policy on seed development; Soil- soil reclamation, alkali soil, saline soils, methods for soil reclamation; Irrigation Environmental degradation and Irrigation projects.

Unit: IV Fertilizers

4. 1 Fertilizers: Effect of Nitrogen, potassium and phosphorous on plant growth. Secondary nutrients – micronutrients- their functions in plants classification of fertilizers, natural fertilizers, artificial fertilizers, phosphate fertilizers; Manufacture of urea and triple super phosphate

4. 2 Manures: Bulky organic manures- Farm yard manure- handling and storage, oil cakes. Blood meal, fish manures.

Unit: V Pesticides and Insecticides

5.1 Pesticides; Classification of Insecticides, fungicides herbicides as organic and inorganic, general methods of application and toxicity, safety measures when using pesticides.

Insecticides: Plant products-Nicotine, pyrethrin, Inorganic pesticides-borates organic pesticides - D.D.T and BMC.

5. 2 Fungicide and Herbicides

Fungicide: Sulphur compounds, copper coumpounds, Bordeaux mixture,

Herbicides: Acaricides- Rodenticides, Attractants- Repellants, Preservation of seeds.

Books Recommended:

1. N.C. Brady, The nature and properties of soils, Eurasia publishing House, New Delhi. 1977.
2. V.S, Jones. Fertilizers and soil fertility, Prentice Hall of India, New Delhi, 1993.
3. D.E.H. Freer, Chemistry of pesticides, D. Van Nostrand Co, Reinhold, 1969.
4. A.K. De. Environmental Chemistry, Wiley Eastern. 1989.
5. A. Sankara. Soils Science.
6. R.C. Palful. K. Goel. R.K. Gupta, Insecticides, Pesticides and Agro based Industries.
7. B.K. Sharma, Industrial Chemistry.

Stereochemistry and organic reactions

Programme:M. Sc., Chemistry Part: Core – I
Semester: II Hours: 5
Subject Code: 17PCHC21 Credits: 4

Course Outcomes

Recognise stereochemistry, conformation and mechanisms of organic reactions and terpenoids and vitamins.

Unit I: Stereochemistry II

Prochirality and prostereoisomerism, enantiotopic and disatereotopic ligands and faces and their nomenclature – pro-R and pro-S and Re and Si faces. Stereospecific and stereoselective reactions.Asymmetric synthesis; Cram's rule and Prelog rules.Optical isomerism due to axial chirality – biphenyl, allenes and spiranes. Molecules with planar chirality- paracyclophanes, transcyclooctene and ansa compounds.

Unit II – Conformational analysis

Configuration and conformation – conformations of ethane and n-butane – conformation analysis – stereo-electronic and steric-factors – conformation of simple acyclic compounds – conformation of monosubstituted and disubstituted cyclohexane – correlation of the conformation of acyclic and cyclic systems with their physical and chemical properties – conformational free enery – Curtin- Hammett principle- Quatitative treatment of mobile system – Eliel-Ro equation – conformation and reactivity of cyclohexanones.

Unit III: Addition to multiple bonds

Electrophilic, nucleophilic and free radical additions – addition to conjugated systems – orientation of the addendum – stereochemical factors in reactions like addition of hydrogen, halogen, hydrogen halide and hypohalous acids. Hydroboration and hydroxylation – epoxidation.

Addition to carbonyl groups – mechanism – Perkin reaction- Knoevenagel reaction- Mannich reactions – Claisen ester condensation – Darzen's reaction – Reformatsky reaction – Wittig reaction- Grignard reactions.

Addition to α, β-unsaturated carbonyl groups – addition of Grignard reagent to α, β-unsaturated carbonyl compounds – Michael addition – Diels- Alder reaction. – addition to carbenes and carbenoids to double bond.

Elimination: α-elimination - β-elimination – E_1 and E_2 and E_1CB mechanisms- orientation of the double bond - Elimination vs. Substitution- pyrolyticcis elimination- Bredt's rule.

Unit IV:

Terpenes:

Classification of terpenoids-structure, stereochemistry and synthesis of α-pinene, camphor, zingeberene, and abietic acid.

Vitamins:

Structure and synthesis of Vitamins A, B1, B2, B6 and B12 (Structural features only) C, E, and H.

Unit V:

Aromatic electrophilic substitution – orientation –reactivity-mechanism of nitration, halogenations, Friedel-Craft's reaction and sulponation –partial rate factors- ortho/para ratio – Quantitative treatment of reactivity of reactivity of the electrophile (the selectivity relationship) – Aromaticnucleophilic substitution reactions - S_NAr, S_N1 and benzyne mechanisms.

Quantitative treatment of the effect of structure on reactivity – The Hammett relationship – significance of reaction and substituents constants – application of the Hammett equation in reaction mechanism –limitations and deviations.

Books Recommended:

1. E. L. Eliel, S.H. Wilen& L.N. Mander, Stereochemistry of carbon compounds, John Wiley & Sons, 2003.
2. V.M. Potapov, Stereochemistry, MIR Publishers, Moscow, 1979.
3. I.L.Finar, Organic Chemistry, vol. II, 5thedn. ELBS, 1975.
4. D. Nasipuri, Stereochemistry of organic compounds. Principles and Applications, New Age International (P) ltd., 2ndedn. 1994.
5. P.S. Kalsi, stereochemistry, conformation and mechanism, New Age international (p) ltd., 4th 1997.
6. T.H. Lowry and K. S. Richardson, Mechanism and Theory in Organic Chemistry.
7. E.S. Gould, Mechanism and Structure in Organic chemistry, Henry Holt & Co., New York, 1959.
8. Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 4thedn., 2000.
9. Reinhard Bruckner, Advanced organic chemistry, Reaction mechanism, Academic press, 2002.
10. F. A. Carey and R.J. Sunderberg, Advanced Organic chemistry, part B, 4thedn., Plenum Publishers, 2001.
11. Paul de Mayo, chemistry of Terpenoids, vol. I & II, academic Press.
12. L. Fieser and Mary Fieser, Steroids, Methuen & Co., New York, 1965.
13. S.F. Dyke, Chemistry of vitamin, Interscience Publishers, 1965.

Coordination and organometallic chemistry

Programme:**M. Sc., Chemistry** Part: **Core – II**

Semester: **II** Hours: *5*

Subject Code: **17PCHC22** Credits: *5*

Course Outcomes

Ascertain bioinorganic compounds and mechanisms of inorganic complexes.

Unit I: Coordination compounds

IUPAC Nomenclature of coordination compounds- isomerism in coordination compounds –Types of ligands –monodentate , ambidentate and macro cyclic ligands – Stability constants – Factors affecting Stability constant in solution – Determination of Stability constant Spectrophotometric method.

Theories of bonding – VB –CFT – MO theories – Splitting of d-orbitals in Octahedral, Tetrahedral and Square planar geometries –CFSE calculation in terms of Dq-Factors affecting crystal field splitting – Spectrochemical series –Magnetic properties of transition metal complexes – Calculation of spin-only magnetic moments.

Unit II: Reaction mechanism of coordination compounds

Substitution reactions of octahedral complexes – labile –inert complexes – mechanisms of acid hydrolysis –base hydrolysis and anation reactions. Substitution reactions of Square planar complexes– The trans effect and its applications – electron transfer reactions – complexomentaryreactions – outer sphere and inner sphere electron transfer mechanism – Synthesis of coordination compounds using electron transfer and substitution reactions.

Unit III: Bioinorganic chemistry I

Porphyrin ring system – metalloporphyrins –hemoglobin and myoglobin structures and work functions – synthetic oxygen carriers –cytochromes – structures and work functions in respiration – chlorophyll- structure – photosynthetic sequence –iron-sulphur proteins (non-heme iron protein) – Copper containing proteins – classification – blue copper proteins – structure of blue copper electron transferases – copper proteins as oxidases –cytochrome C oxidase – mechanism studies of C oxidase – Hemocyanin.

Unit IV: Bioinorganic chemistry II

Carboxypeptidase A: structure, function – carbonic anhydrase – inhibition and poisoning – corin ring system-vitamin B_{12}coenzyme –in-vivo and in-vitro nitrogen fixation – essential and trace elements in biological systems – metal ion toxicity and detoxification –molecular mechanism of ion transport across the membrane – sodium and potassium ions pumps –chelate therapy – *cis*-platin.

Unit V: Complexes of π-acceptor ligands

Synthesis, structure and bonding in metal carbonyls and nitrosyls complexes-Application of EAN rule.

Synthesis properties, structure and bonding in Ferrocene, acetylene and allyl complexes.

Catalysis using organometallic compounds:

Oxidative addition – reductive elimination –insertion reaction-Catalytic mechanism in the following reactions-hydrogenation of olefins (Wilkinson catalytic) -hydroformylation (oxo process) - oxidation of alkenes to aldehydes and ketones (Wacker process)- catalysis in the formation of synthesis of gas-olefin polymerization (Ziegler-Natta) – Cyclo oligomerization of acetylenes (Reppe's catalyst or Wilke's catalyst) Olefin isomerization using Ni catalyst.

Books Recommended:

1. W. E. Addison, Structural Principles of Inorganic Chemistry, Wiley, 1961.
2. A.F. Wells, Structural Inorganic Chemistry, 4th Ed, Oxford, New York, 1975.
3. F.A. Cotton and G. Wilkinson, Advances Inorganic Chemistry, 5th Ed, John Wiley & Sons, Singapore, 1988.
4. K.F. Purcell and J.C. Kotlz. An Introduction to Inorganic Chemistry, W. B. Sanders. Company, Philadelphia. 1980.
5. James E. Hugheey, Ellen A. Keitler and Richard, L. Keitler, Inorganic chemistry, 4th Ed, Harper Collins college Publishers. New York, 1993.
6. Y. Mido, Chemistry in Aqueous and nonaqueous solvents, Discovery publishers house, NewDelhi, 1969.

Group theory and spectroscopy

Programme: **M. Sc., Chemistry** Part: **Core – III**

Semester: **II** Hours: *5*

Subject Code: **17PCHC23** Credits: 4

Course Outcomes

Illustrate group theory and spectroscopy.

Unit I: Group Theory

Molecular Symmetry elements and symmetry operations- Matrices-Matrix representation of symmetry operations and transformation matrices- Group- definition and properties of a group- Symmetry point groups- representation of a group- reducible and irreducible representations- Great orthogonality theorem- characters- construction of character tables- C_{2V}, C_{3V}, C_{4V} and D_{2d}- Direct product concept.

Unit II: Application of Group Theory to spectroscopy and Molecular Problems

Symmetry of normal modes of vibrations, application of group theory to normal modes of vibrations and to normal mode analysis- Symmetry properties of integrals- application for spectral selection rules of vibration spectra- IR and Raman active fundamentals. Symmetry of molecular orbitals and Symmetry selection rules for electronic transitions in simple molecules like ethylene, formaldehyde and benzene. Group theory and quantum mechanics- wave functions as the basis of irreducible representations- Group theory applied to hybridization- HMO theory- HMO calculations and delocalization energy for cyclopropenyl, butadiene and benzene systems.

Unit III: Molecular Spectroscopy I

Electromagnetic spectrum- Types of molecular energies- Absorption and emission of radiation- Einstein's coefficient- induced emission and absorption- Rotational spectra of rigid diatomic molecules- isotope effect in rotational spectra- Microwave spectrometer-Informations derived from rotational spectra.

Infrared spectroscopy- vibrational energy of a diatomic molecule- Infrared selection rules- diatomic vibrating rotator- vibrations of polyatomic molecules- overtone, combination and difference bands- concept of group frequencies- coupling interaction- Fermi resonance- Fourier transform infrared spectroscopy.

Unit IV: Molecular Spectroscopy II

Raman spectroscopy - Theories of Raman scattering- Rotational-vibrational Raman spectra- Mutual exclusion principle- Laser Raman spectra- Electronic spectra of diatomic and polyatomic molecules-intensity of vibrational electronic spectra- Franck-Condon principle- rotation fine structure of electronic vibrational spectra- the Fortrat parabola- Dissociation and predissociation spectra.

NQR- principles and applications- quadrupole moment and electric field, nuclear quadrupole resonance, nuclear quadrupole coupling in atoms and molecules.

Unit V: Spin Resonance Spectroscopy

Magnetic properties of nuclei- Resonance condition- NMR instrumentation- Relaxation processes- Bloch equations- chemical shift- spin-spin splitting, relaxation times, line shape and line width experimental techniques- double resonance techniques, ENDOR, Overhauser effect, FT-NMR spectroscopy, Lanthanide shift reagents- NMR imaging.

ESR- principles of ESR- Total Hamiltonian-hyperfine structure- ESR spectra of free radicals in solution- Anisotropic systems-systems in triplet state- Zero field splitting in ESR and Krammer's degeneracy.

Books Recommended:

1. F.A.Cotton, Chemical Applications of Group Theory, 3nd Edn., John Wiley & Sons, New York (1999).
2. G.Davidson, Introduction to Group Theory for chemist, Applied Science Publishers Ltd, London(1971).
3. V. Ramakrishnan and Gopinath, Group Theory in Chemistry, 2nd edn.,Vishal publications,1991.
4. K.V.Raman, Group Theory and its application to chemistry. Tata McGraw-Hill (1990).
5. A. Streitweiser, Molecular Orbital Theory for Organic chemistry,John Wiley & Sons.
6. C.N.Banwell and E.M.Mccash, Molecular Spectroscopy, Tata McGraw-Hill,4th Edn.,(1995).
7. G. Arulhas, Molecular Structure and Spectroscopy, Prentice- Hall of India Pvt.,Ltd, New Delhi(2001).
8. R. S. Drago, Physical Methods in Chemistry, W.B. Saunders Co., London (1977).
9. D.C.Harris and M.D. Bertolucci, Symmetry and Spectroscopy- An introduction to vibrational and electronic Spectroscopy, Oxford University Press, New York (1978).
10. G.H. Barrow, Introduction to Molecular Spectroscopy, McGraw-Hill.
11. R.Chang, Basic principles of Spectroscopy, McGraw-Hill, London (1976).
12. B.F.Straughan and S.Walker(eds), Spectroscopy, Vol 1,2 and 3,chapman & Hall, London(1976).
13. P.W.Atkins, Physical Chemistry, 6th edn., Oxford University Press, Tokyo (1998).
14. E.B.Becker, High Resolution NMR, 2nd edn.,Academic Press,1990.
15. A.Carrignton and A.D. McLachian, Introduction to Magnetic Spectroscopy, Harper and Row.
16. D. Shaw, Fourier Transform NMR Spectroscopy, Elsevier.

Semester II

Organic chemistry practical

17PCHC2P	Organic qualitative and quantitative analyses and preparations	Hours 10/Credits 5

Separation and analysis of two component mixtures. Identification of the components and preparation of solid derivative.

1. Quanitative analysis:

a. Estimation of glucose by lane and eynon method and Bertrand method
b. Estimation of glycine
c. Estimation of formalin
d. Estimation of methyl ketone

2. Organic preparations: (only for class work)

About 3 (five) two-stage preparation:

a. P-Nitro aniline from acetanilide benzophenone
b. P-Bromo aniline from acetanilide Aniline
c. m-Nitro benzoic acid from methyl benzoate.

Analytical chemistry

Programme: **M. Sc., Chemistry** Part: **Elective – I**

Semester: **II** Hours: *5*

Subject Code: **17PCHE21** Credits: *5*

Course Outcomes

Elicit electro analytical, thermo analytical and spectro analytical methods.

Unit I: Precipitation Techniques

Introduction –properties and precipitating reagents-Colloidal precipitates-Co-precipitation –Post-precipitation –Precipitates from homogenous solutions – Surface adsorption –Drying and ignition of precipitates – Application of gravimetric methods.

Unit II: Error Analysis

Error analysis: Classification of errors –accuracy and precision –minimization of errors – significant figures – significant figures in computation – statistical treatment of data- mean, median, standard deviation, variance, relative standard deviation –spread, errors – standard deviation of computed results-reliability of results-Q test, T-test – confidence limit-comparison of results- Student's test –F-test T-test – comparison of the means of two samples- correlation and regression: linear regression (least square analysis).

Unit III: Electroanalytical Methods

Electro analytical Techniques: Electrogravimetry: Theory of electrogravimetric analysis - Electro analytical separation and determination of metal ions, Coulometry: Electrolytic cell - work electrodes - auxilliary electrode and reference electrode – Coulometric titrations. Voltammetry - Cyclic voltammetry – stripping voltammetry – chromopotentiometry - Amperometry; Amperometric titrations.

Unit IV: Thermoanalytical Methods

Thermal analysis; Theory and principles of DTA and TGA – factors affecting the position of DT and T G traces- application of DTA and TGA to the thermal behavior of the following compounds- crystalline copper sulphate, calcium oxalate monohydrate, calcium acetate monohydrate, - Comparison of DTA and TGA –

principle and application of DSC –determination of degree of conversion of high alumina cement.

Unit-V: Spectroanalytical methods

Colorimetry:

Beer and Lambert's law – terminology – conditions for a satisfactory colorimetric analysis – methods of colour measurement or comparison - principles of colorimetric determinations of Cr, Fe, Mn - simultaneous spectrophotometric determination of Cr and Mn.

Nephelometry and turbidometry:

Determination of sulphate and phosphate.

Fluorimetry:

Principle – application of flourimetry in the determination of Ca, Cd and Zn and determination of codeine and morphine in a mixture.

Flame spectrometry:

Theory – interferences – AAS - applications in the determination of Mg^{2+}, Ca^{2+} in tap water.

Books Recommended:

1. D. A. Skoog, D. M. West and F. J. Holler, Fundamentals of Analytical Chemistry, 7th Edition, Saunders College Publishing, Philadelphia, 1996.
2. Willard HH, Merritt LL, Dean JA, Settle PA. Instrumental Methods of Analysis, 6th Ed. New York: Van Nostrand, 1988.
3. J. Basset et al., Vogel's Text book of Qualitative Inorganic Analysis, Longman, 5th Edition, ELBS, Essex, 1989.
4. J. G. Dick, Analytical Chemical, Tata-McGraw Hill, 1973.

INDUSTRIAL CHEMISTRY

Programme:**M. Sc., Chemistry** Part: **Elective – II**

Semester: **II** Hours: *5*

Subject Code: **17PCHE22** Credits: *5*

Course Outcomes

To gain knowledge about glass and ceramics, cement, dyes and paints, plastics, oils, and fats.

Unit: I Glass and Ceramics

1.1. Glass: Introduction. Raw materials, manufacture and applications. Some special glasses-fused silica glass, optical glass, glass wool, photosensitive glass-composition and uses.

1.2. Ceramics: Definition. Manufacture and applications.

Unit: II Cement

Introduction, Types of cement- High alumina cement, Slag cement, Acid resisting cement, White cement, Types of Portland cement, Raw materials, Manufacture of cement, Setting of cement, factors affecting quality of cement, Cement industries in Tamilnadu.

Unit: III Dyes and Paints

3.1. Dyes: Classifications of dyes, application of dyes in other areas-medicine, chemical analysis, cosmetics, colouring agents, Food and beverages.

3.2. Paints: Constituents of paints, Manufacture of paints, Setting of paints, requirement of a good paint, paint failure.

Unit: IV Synthetic fibres and Plastics

4. 1. Synthetic fibres: Difference between natural and synthetic fibres, Applications of synthetic fibres-Rayon, Terylone, Nylon. Taflon.

4 . 2. Plastics: Domestic and industrial applications of all types of plastics.

Unit: V Oils, Fats and Waxes

Classification of oils, fats and waxes, distinction between oils, fats and waxes, Uses of essential oils and fats. Soap and its manufacture toilet and transparent soaps cleansing action of so ap Detergent – classification and uses.

Books Recommended:

1. B.K. Shanna, Industrial Chemistry, Goel Publishing House Pvt Ltd. 1999.
2. M.G. Arora and M. Sin«h, Industrial Chemistry. Anmol Publications, 1st edition, 1994.
3. G.N.Pandey, A Textbook of Chemical Technology. Vol. I and I I, Vikas Publishing House Pvt Ltd. 1997.
4. B.K. Chakrabarty, Industrial Chemistry, Oxford & IBM Publishing CO. Pvt Ltd. 1991.
5. V. Subrahmaniyan, S. Renganathan. K.Ganesan, S.Ganesh. Applied Chemistry. Scitcch Publications, 1998.
6. J.E.Kuria Cose and J.Rajaram, Chemistry in Engineering & Technology. Vol.1 I I , T a t a Mc Craw Hill. 1984.

Organic spectroscopy and natural products

Programme: **M. Sc., Chemistry** Part: **Core–I**

Semester: **III** Hours: *5*

Subject Code: **17PCHC31** Credits: 4

Course Outcomes

Classify different organic spectroscopic and analytical methods in organic compounds and about steroids, also about certain alkaloids and antibiotics.

Unit I: Spectroscopy I

UV Spectroscopy: Principle – absorption spectra of conjugated dienes - α, β-unsaturated carbonyl compounds- Woodward-Fieser rules.

IR Spectroscopy: Molecular vibrations – vibrational frequency – factors influencing vibrational frequencies.

Mass Spectroscopy: Principle – Type of ions – Parent ion , meta stable and isotopic peaks – Nitrogen rules – Pattern of fragmentation for various classes of compounds - McLafferty rearrangement – Retro Diels-Alder reaction.

Unit II: Spectroscopy II

H^1 NMR Spectroscopy:

Introduction of NMR spectra – chemical shift – spin-spin coupling – coupling constant- first and second order spectra– factors influences on chemical shift or protons- simplification of complex spectra- deuterium substitution – spin decoupling – double resonance – shift reagents – Nuclear overhauser effect – CIDNP-NMR concept of aromaticity.

C^{13} NMR Spectroscopy:

Basic principle of FT technique – Relaxation time – assignment of signals – Off resonance decoupling - calculation of chemical shifts for aromatic and aliphatic compounds – DEPT ^{13}C spectra - ^{13}C-^{13}C correlation COSY, HETCOR, ROESY, and NOESY - technique.

Unit III: Chiro optical and Analytical techniques

ORD and CD – Principle- cotton effect- type of ORD curves- α-halo ketone rule- octant rule- applications to determine the configuration and conformation of simple mono cyclic and bi cyclic ketone and comparison of ORD and CD.

Chromatographic techniques: Column- TLC, paper, GLC, HPLC, exclusion and ion exchange.

Unit IV:

Steroids: Classification – Complete chemistry of cholesterol (includes bile acids) chemistry of Ergosterol and Vitamin D_2 – Male sex hormones – Androsterone – Testosterone- Female sex hormone- Oestrone, Equilenin and Progesterone – a basic idea about adrenocortical hormones – cortisone (synthesis not included)

Prostaglandins: General study of prostaglandins- structure – Chemistry of PGE1.

Unit V:

Alkaloids: General methods of structural determination – Hoffmann, Emde and Von Braun degradations. Structure and synthesis of quinine, norcotine, morphine.

Antibiotics: Definition, classification of antibiotics, structure, stereochemistry and synthesis of penicillin, chloramphenicol, Terramycin.

Books Recommended:

1. John R. Dyer. Application of adsorption Spectroscopy, Prentice- Hall.
2. William Kemp, Organics Spectroscopy. ELBS, 3rdEdn.
3. Robert M. Silverstein, Francis X. Webster, Spectrometric Identification of Organic compounds, 6thEdn., John Wiley & Sons, Inc., 2004.
4. I. L. FInar, Organic chemistry, Vol. II. ELBS, 1975.
5. Paul de Mayo, Chemistry of Terpenoids, Vol. I &Vol II, academic Press.
6. L. Fieser and MayrFieser, Steroids, Reinhold, 1953.
7. W. Klyne, The chemistry of steroids, Methuen & Co., Newy York, 1965.
8. E.L. ELiel, Stereochemistry of carbon compounds, McGraw Hill, 1962.
9. P. Crabbe, ORD and CD in chemistry and Biochemistry, Academic Publishers 1972.
10. A, Brainth Waite and F.J. Smith. Chromatographic Methods, Chapman and Hall., 4thEdn. 1985.
11. K.W. Bently, Alkaloids, Vol I & II, Intersicence, 1957.

Inorganic spectroscopy and nanotechnology

Programme: **M. Sc., Chemistry** Part: **Core-II**

Semester: **III** Hours: *5*

Subject Code: **17PCHC32** Credits: 4

Course Outcomes

To understand the Rearrangement mechanisms, shift reagents. To grow their spectroscopic knowledge about how to find out the NMR, ESR, IR, UV active compounds. To compare the orbital degeneracy of various molecules.

Unit I: Electronic spectra of transistion metal complexes and photochemistry

d-d transition-charge transfer transistion-selection rules-mechanism of breakdown of selection rules-bandwidths and shapes-John Teller effect-Tanabe-sugano Diagram-evaluation of 10Dq and β for Octahedral and Tetrahedral complexes of d^1 to d^9 configurations-Photochemistry-photoredox and substitution reactions occurring in Co(III) and Cr(III) complexes-photochemistry of ruthenium polypyridyls.

Unit II: Application of Spectroscopy to the study of Inorganic compounds I

Application of IR and Raman spectra in the study of coordination compounds-application to metal carbonyls and nitrosyls-geomentrical and linkage isomerism-strectching mode analysis of metal carbonyls.

Mossbauer spectroscopy: Mossbauer Effect resonance absorption-Doppler effect – Doppler velocity– Isomer shift-magnetic hyperfine splitting –application of Mossbauer spectroscopy in the study of Iron and Tin complexes.

Photoelectron spectroscopy (PES): Chemical identification of elements – Koopmann's theorem – chemical shift– spin- orbit coupling –Auger spectroscopy – principles and its applications.

Unit III: Application of spectropscopy to the study of Inorganic compounds II

NMR Spectroscopy:

^{31}P - ^{19}F and ^{15}N –NMR –Introduction-applications in structural in problems– NMR of Fluxional molecules –NMR of paramagnetic molecules –contact shifts and shifts Reagents.

ESR spectroscopy:

Principles –presentation of the spectrum –hyperfine splitting –factors affecting magnitude of g values –zero field splitting –Kramer's degeneracy-ESR of d^3Octahedral complexes –anisotropy –hyperfine splitting constants-application of

ESR in the study of transition metal complexes – John Teller distortion studying in Cu(II) complexes – Evaluation of spin orbit coupling

Unit IV: Nano chemistry

Basic Idea of Nano chemistry – Definitions in Nano technology – Size of Nano –Techniques of Methodology.

Fullerenes: Introduction – Properties.

Nano particles: Introduction – Properties – Classifications – Production.

Nano tubes: Structure and characterization single walled carbon nano tubes –Nano tubes properties –applications of Nano tubes.

Nano structured Polymers: Conducting polymers –block –copolymers-Nano cages.

Unit V: Molecular Rearrangements and reaction of coordinated ligands

Molecular rearrangement of four coordinated complexes –six coordinated complexes-reation at coordinated ligands-reaction due to metal ion polarization of coordinated ligands-hydrolysis of amino acids –esters , amides and of peptides-Aldol condensation –Imine formation –hydrolysis and substituent exchange-the template effect and Macrocyclic ligands.

Books Recommended:

1. F. Basalo and R.G. Pearson, Mechanism of Inoganic reaction, 2nd Edn., Wiley, New York, 1967.
2. Adamson, Concept of Inorganic Photochemistry, Wiley, New York, 1975.
3. S.F. Kettle, Coordination chemistry. An approach, Spectrum Academic Publishers, Oxford, 1996.
4. R.S. Drago, Physical Methods in chemistry, Sanders Golden Sunburst series, W.B. Saunders company, London, 1977.
5. I. Bertini et al. Bioinorganic chemistry, Viva Books Pvt Ltd, Chennai, 1998.
6. ChatwalBhagi and Agarwal, Bioinorganic chemistry, sultan chand co., New delhi, 2001.
7. M.A. O. Hill and P. Day (Eds), Physical Methods in Advanced Inorganic chemistry, Interscience, Newyork, 1968.
8. R. S. Drago, Physical Methods in Chemistry, W.B. Saunders Co., London (1977).
9. K.F. Purcell and J.C. Kotlz. An Introduction to Inorganic Chemistry, W. B. Sanders. Company, Philadelphia. 1980.

Semester III

Physical chemistry practical

17PCHC3P	Conductometric and potentiometric titrations and kinetic, adsorption and spectral measurements	Hours 10/Credits 5

I. Conductometric experiments

i. Double displacement & acid base titrations

a) NH_4Cl → NaOH → Mixture of CH_3COOH & HCL

b) NH_4Cl → NaOH → Mixture of NH_4Cl & HCL

ii. Precipitation titration

a) Na_2CO_3 → $Pb(NO_3)_2$ → Na_2CO_3

b) K_2SO_4 → $BaCl_2$ → K_2SO_4

II. Adsorption experiments

Adsorption of oxalic acid/acetic acid on charcoal

III. Kinetic experiments

i. Kinetics of alkali hydrolysis of ester by potentiometric method.

ii. Per disulphate and iodide ion reaction : Study of primary salt effect and determination of the concentration of given KNO_3.

IV. Potentiometric methods

i. Precipitation titration: Ag+ Vs halide mixture

ii. Redox titrations: a) Permanganate Vs iodide ion

b) Ceric ammonium sulphate Vs ferrous ion

iii. Determination of dissociation constant of weak acids and pH of buffer solutions

iv. Determination of solubility product of sparingly soluble salts.

V. Titrations using P^H meter

Determination of first, second and third dissociation constants of phosphoric acid.

VI. Experiments based on UV-Visible and Infra-red spectrophotometers.

Quantum, Nano and Macromolecular Chemistry

Programme: **M. Sc., Chemistry** Part: **Elective –I**
Semester: **III** Hours: *5*
Subject Code: **17PCHE31** Credits: *5*

Course Outcomes

Formulate Quantum mechanics frame works and instrumentation in nano science.

Unit I: The Birth of quantum mechanics Plank's explanation about black body radiation

Debroglie concept of matter waves, Compton effect- Heisenberg's uncertainty principle - operators- linear operator – method of getting the following quantum mechanical operator- position, momentum, kinetic energy, potential energy, total energy, angular momentum.

Postulates of quantum mechanics- hermicity and proving the quantum mechanical operators are hermitian- commutators – eigen function and eigen value- introducing dirac notation. Orthogonality and normalization of wave function.

Unit II: Application of quantum mechanics to simple systems

Derivation of schrodinger wave equation – free particle moving in one dimensional box- physical interpretation of the one dimensional problem- characteristics of wave function- average momentum of a particle in a box is zero- particle moving in 3-D box- degeneracy – distortion – particle moving in a ring- rigid rotator – spherical harmonics- simple harmonic oscillator - hydrogen atom problem- radial wave function- radial probability distribution – shapes of various atomic orbitals- Term symbols- LS couplingscheme- spectroscopic states.

Unit III: Approximation methods in quantum mechanics

Need for approximation methods- schrodinger equation for He atom and other many electron system- the time independent perturbation theory(first order only)- application to hydrogen atom- variation theorem- application to hydrogen and helium atom- Hartee- fock- self consistent field (HFSCF) method of many electron system and its application to helium atom- electron spin and pauli's principle-antisymmetric nature of the wave functions- Slater determinants- electronic configuration of many electron system- Born-Open heimer approximation –VB and MO theories, MO treatment of hetero nuclear and homo nuclear diatomic molecules.

Unit IV: Instrumentation in Nano chemistry

Microscopic techniques for the characterization of nano materials- Fluorescence spectroscopy- AFM, SEM, TEM, X-RAY diffraction and micro analysis.

Unit V: Macromolecular chemistry

Macro molecules over view of polymers- types and properties of polymers- kinetics and mechanism of free radical, ionic , condensation and Zeigler-Natta polymerization process- emulsion and suspension polymerization techniques- polymer molecular weight and its distribution- molecular weight determination- osmotic pressure method- light scattering g method- ultra centrifuge method and viscosity method-conducting polymers.

Books Recommended:

1. A. K. Chandra, Introductory Quantum Chemistry, 3rdEdn., Tata McGraw Hill Publishing Co., New Delhi, 1988.
2. M.W. Hanna, Quantum Mechanics in Chemistry, 2ndEdn., The Benjamin/Cummings publishing Co., London, 1969.
3. D.A. McQuarrie, Quantum Chemistry, 1st Indian Edn., Viva Books Pvt Ltd, New Delhi, 2003.
4. P.W. Atkins, Molecular Quantum Mechanics, 2ndEdn., Oxford University Press,, 1986.
5. C.P. Poole and F.J. Owens. Introduction to nanotechnology, 2004.
6. C.C. Koch Nano structured Materials.

Environmental Science

Programme: **M. Sc., Chemistry** Part: **Elective –II**

Semester: **III** Hours: *5*

Subject Code: **17PCHE32** Credits: *5*

Course Outcomes

To study the types of pollution, pollutants and measurement of pollutants.

Unit I: Introduction and classification

Introduction- Environmental Science- Environmental chemistry-Ecology-Definition-Eco System-Cycling of mineral elements and gases-phosphate cycle-Carbon cycle-Hydrogen cycle-Nitrogen cycle-Hydrological cycle- Environmental segments-pollution and its types: air pollution-water pollution-soil pollution-radioactive pollution-thermal pollution-noise pollution-marine pollution-other types of pollution- and its effects and control- remedial measures.

Unit II: Air pollution

Introduction-sources of air pollution-air pollutants-classification and effects of air pollutants-oxides of nitrogen, sulphur and carbon-acid rain-effects and control-hydrogen sulphide-effects and control- carbon mono oxide-effects and control-photochemical smog- effects and control- fly ash- effects and control- green house effects-global warming-effects and control-ozone layer-ozone depletion-chlorofluoro carbons--effects and control.

Unit III: Water pollution

Introduction-types of water- Water pollution-sources of water pollution-water pollutants-classification-physical,chemical and biological-inorganic pollutants and toxic metals-organic pollutants-radioactive pollutants in water- pesticides and fertilizers- suspended particles- water quality-water quality index- ill effects of water pollutants-fluorosis-water pollution control- water treatment- primary, secondary and tertiary treatment-desalination-reverse osmosis-sewage and industrial waste water treatment.

Unit IV: Soil pollution

Introduction-types of soil- Soil pollution-types-indicators of Soil pollution-plants as indicators of pollution-sources of Soil pollution- fertilizers and pesticides-radioactive pollutants- solid wastes- soil sediments as pollutant-soil erosion-treatment of soil pollutants-treatment of solid wastes- thermal methods-land filling-composting- land protection-remedial measures for Soil pollution.

Unit V: Analysis of pollutants

Introduction- analysis of air pollutants- units-sampling-devices and methods for sampling-measurement: UV-Visible spectrometry-IR spectrometry- emission spectrometry - turbidimetry, nephelometry - gas chromatograpy – HPLC - chemiluminescence of nitrogen oxides - IR photometry – conductometry - analysis of water pollutants-units-sampling- devices and methods for sampling- measurement: UV-Visible spectrometry-titration-analysis of different water quality parameters-BOD- COD analysis and monitoring of pesticides, carcinogens and industrial pollutants.

Books Recommended:

1. B.K.Sharma and H. Kaur, Environmental chemistry,Krishna Prakashan,Meerut,1997.
2. A. K. De, Environmental chemistry,Wiley Eastern Ltd., Meerut,1994.
3. A. K.Mukherjee, Environmental pollution and Health Hazards- causes and control, Galgotia press, New Delhi, 1986.
4. N. Manivasakam,physio-chemical Examination of water, Sewage and Industrial Effluents, Pragati Prakashan Publ., Meerut, 1985.

Applications of chemistry

Programme: M. Sc., Chemistry Part: NME

Semester: III Hours: 5

Subject Code: 17PCHN31 Credits: 5

Course Outcomes

To know the structure of atom, organic chemistry and purification of organic compounds. To study about vitamins, alkaloids and antibiotics. To understand acids and bases. To study about colloids and hardness of water. To study different types of polymers.

Unit I: Introduction

Definition of Organic Chemistry – Comparison of organic and inorganic compounds – Molecular formula – Purification of Organic compounds – Distillation – Isomerism – Structural isomerism only.

Unit II: Polymer

Polymers – classification of Polymers – preparation and uses of polyethylene, PVC, Teflon, Polystyrene, Dacron and Nylon 6, 6 – Natural rubber – Synthetic rubber – Neoprene rubber – Styrene – Butadiene rubber(SBR).

Unit III: Vitamins, alkaloids and antibiotics

Vitamins – classification – Structure, sources and functions of Vitamins A, B, C, D, B2 and B6 – Antibiotics – classification of antibiotics – alkaloids - classification of alkaloids – occurrence and extraction – General properties of alkaloids.

Unit IV: Acids and bases

Bronsted – Lowry concept, Lewis concept, Arrhenius concept of acids and bases – P^H Scale – Buffer solutions – Acid – base Indicators – Action of Phenolphthalein and methyl orange.

Unit V: Colloids and hardness of water

Colloids – classification – Purification of Colloids – Dialysis and ultrafiltration – Electro kinetic Properties – electrophoresis & electro osmosis – applications of Colloids – Hardness of water – types of hardness – estimation of hardness by EDTA method.

Books Recommended:

1. I. L. FInar, Organic chemistry, Vol. II. ELBS, 1975.
2. K.W. Bently, Alkaloids, Vol I & II, Intersicence, 1957.
3. S.F. Dyke, Chemistry of vitamin, Interscience Publishers, 1965.
4. B. R. Puri, L. R. Sharma and M.S. Pathania, Priciples of Physical chemistry (MilleniumEdn) Vishal Publishing Co., (2003)
5. V.R. Gowariker, N.V. Viswanathan and JayadevSreedher, "Polymer Science", Wiley Eastern Ltd., New Delhi 1986.
6. B.K. Sharma, "Polymer Chemistry", Goel Publishing House, Meerut, 1989.
7. ArunBahl, B.S. Bahl, "A Text Book of Organic Chemistry" S. Chand & Company Ltd.

Biomolecules, photochemistry, rearrangement and synthetic methods

Programme: **M. Sc., Chemistry** Part: **Core-I**

Semester: **IV** Hours: *5*

Subject Code: **17PCHC41** Credits: *4*

Course Outcomes

Distinguish amino acids, carbohydrates, mechanism in molecular rearrangements and green chemistry and micro wave synthesis.

Unit I: Proteins, amino acids, Nucleic acids and Carbohydrates

Classification of proteins – peptides – structure of peptides- synthesis of peptides – chemistry of glutathione and oxytocin – an elementary treatment of enzymes, coenzymes and nucleic acids- biosynthesis of amino acids.

Introduction to carbohydrates

Pyronose and furanose, forms of aldohexoses and keto hexoses – methods used for determination of ring size – conformation of aldohexopyranoses- structure and synthesis of maltose, lactose sucrose and cellobiose.

Unit II: Pericyclic, photochemical and free radical reactions

Pericyclic reactions:

Conservation of orbital symmetry – electrocyclic reactions – [2+2] and [4+2]cycloaddition reactions-sigmatropicrearrangement (Coperearrangement) – applications of correlation diagram approach, Frontier molecular orbital approach, Huckel-Mobius approach.

Photochemical reactions:

Photochemical reactions of ketones – photosensitization – Norrish I and II type reactions- Patternobuch reactions – Photooxidation – Photoreduction .

Free radical reactions:

Barton, Sandmeyer , Gomberg-Bechmann, Ullmann and Pschorr Hundicker.

Unit III: Molecular rearrangements

Mechanism of the following rearrangement reactions: Wagner-Meerwin, Bechmann, Wolff, Baeyer-villiger, Stevens, Sommellet-Hauser, Favorskii, Benzil-bezillic acid, Fries, Dienone-phenol, di-pi methane, and benzidine rearrangement – Photochemical rearrangement.

Unit IV: Green Chemistry I

Principles of green chemistry – planning a green synthesis in a laboratory – general interest for solvent free processes- Microwave synthesis: Introduction and characteristics of microwave heating – difference between conventional heating and microwave heating. Dielectric poloarization – dipoloar polarization – application and advantages of microwave heating over conventional heating.

Unit V: Synthetic methods

Planning a synthesis – Linear approach and convergent approach to total synthesis – Retro-synthetic analysis of simple organic compounds – Functional Groups Interconversion (FGI) – Activating and blocking groups in synthesis – Umpolung synthesis - Robinson annelation - A schematic analysis of the total synthesis of the following compounds: 2,4-dimethyl-2-hydroxypentanoic acid and Trans-9-methyl-1-decalone.

Books Recommended:

1. A.I. Lehninger, Biochemistry, Nath Publications.
2. C.H. Depuy and O.L. Chapman, Molecular Reactions and Photochemistry, Prentice Hall, 1972.
3. S.M. Mukherji and S.P. Singh, Reaction Mechanism in Organic Chemistry, McMilan India Limited, 1978.
4. R.B. Woodward and R. Hofmann, The Conservation of Orbital Symmetry, VerlogChemie GMBH and Academic Press, 1971.
5. Hung, The Chemistry of Free Radicals.
6. I.L. Finar, Organic Chemistry, Vol. II, ELBS, 1975.
7. P.De. Mayo, Molecular Rearrangements.
8. Jerry March, Advanced Organic Chemistry, John Wiley&Sons, 4thedn., 2000.
9. K.R. Desai, Green Chemistry (Microwave Synthesis) Himalaya Publishing House, Mumbai, 2005.
10. R.Sanghi and M.M. Srivastava, Green Chemistry (Environmental Friendly Alternatives), Narosa Publishing House, India, New Delhi, 2003.
11. A.k. Ahluwalia, Green Chemistry (Environmentally Benign Reactions) Aru Books India, New Delhi 2006.
12. R.E. Ireland, Organic Synthesis, Prentice-Hall of India Pvt. Ltd., 1975.
13. R.D. Morrison and R.N. Boyd, Organic Chemistry, Prentice-Hall, 6thedn., 2001.

Nuclear and analytical chemistry

Programme:M. Sc., Chemistry Part: Core-II

Semester: IV Hours: 5

Subject Code: 17PCHC42 Credits: 4

Course Outcomes

To understand the fission and fusion mechanisms. To grow their computer knowledge about browsing, programming. To know the radioactive element's uses. To compare the processes of Nuclear power reactor and breeder reactor. Classify the various reactors.

Unit I: Structure of nucleus and radioactive decay

Composition of the nucleus-nuclear size,shape and density – principal,radial and magnetic quantum numbers- elementary treatment of shell(independent particle)model –nuclear configuration-parity and its conversion –mass defect and binding energy-nuclear forces theory.

Radioactive decay:

Group displacement law –decay series –rate of disintegration –half life – average life – Units of radio activity - theories of alpha decay,beta decay,gamma emission,positron decay, nuclear isomerism,internal conversion and electron capture.

Unit II: Nuclear fission and fusion and application of radioactive isotopes

Bethe's notation of nuclear process –nuclear reaction energies(Q value)-fission-energy release in nulear fission-mass distribution of fiision products-theory of nuclear fission –fissile and fertie isotopes-energy from nuclear fission – thertmonuclear reactions in stars-classification of stars-power nuclear reactor-breedor reactor –nuclear reactors in india.

Applications of radioactive isotopes:

Characteristics of tracer isotopes – chemical investigations – age determination – medical field –agriculture –industry -analytical applications-isotope dilution analysis-neutron activation analysis –biological effects of radiation-waste disposal management.

Unit III: Lanthanides and Actinides

Chemistry of lanthanides and actinides : Lanthanides –Occurrence, extraction from ores –separation procedure-ion exchange method – solvent extraction method .physical and chemical properties – Electronic configuration -common oxidation state –lanthanide contraction and its consequences- colour of lanthanide ions – magnetic properties of lanthanides-separation of actinide elements - separation of pu from fission products -electronic configuration –oxidation state –comparision of lanthanides and actinides –position in the periodic table.

Unit IV: Electro analytical and thermoanalytical methods

Electrogravimetry:

Theory of electro gravimetric analysis – Electrolytic separation and determination of metal ions. Coulometry - coulometric titrations .Voltammetry :Cyclic voltammetry-stripping voltammetry –chronopotentiometry.Amperometry: Amperometric titrations.

Thermo analytical methods:

Instrumentation and applications of thermogravimetry –Differential Thermal Analysis and Differential scanning colorimetry.

Spectroanalytical methods:

Spectroanalytical methods :Laws of absorption and quantitative law of luminescence –principles and applications of colorimetry and spectrophotometry, fluorimetry, nepheleometry and turbidometry –emission spectroscopy and flame spectroscopy-atomic absorbtion , atomic emission and and atomic fluorescence spectroscopy –Optical rotator dispersion and circular dichorism.

Unit V: Computers in chemistry

History and development of computers, Mainframe ,micro and super computer systems -CPU and other peripheral devices –Evolution of programming language and higher level language .Syntax and structure of C language.

Internet –History of internet –the working of internet and internet services-applications of internet in chemistry –websites in Literature survey in chemistry –popular web sites in chemistry –data base in chemistry –downloading the attachment/ PDF files – opening, browsing and searching a web site –literature searching online.

E-mail: Introduction –working way –mailing basics e-mail ethics –advantages and disadvantages –creating e-mail id –receiving and sending e-mails.

Books Recommended:

1. S. Glasstone, Source Book on Atomic energy, 3rdedn., Van Nostrand Reinhold Company, NewYork, 1967.
2. G. Friedlander, J.W. Kannedy, E.S. Macias and J.M. Miller. Nuclear and Radiochemistry, John Wiley & Sons Inc., New York, 1981.
3. H.I. Arnikar, Essentials of Nuclear Chemistry, 3rdEdn., Wiley Eastern Ltd.
4. U.N. Dash, Nuclear Chemistry, Sultan Chand and sons, New Delhi, 1991.
5. J. Basset et al. Vogel's Text book of Quantitative Inorganic Analysis, Longman, 5thEdn., ELBS, Essex, 1989.
6. H. H. Wilard, LL. Merritt and J.A. Dean, Instrumental Methods of Analysis, East-West Press, New Delhi, 1988.
7. D.A. Skoog and D.M. West, Fundamentals of Analytical Chemistry, Saunders College Publishing Co., Philadelphia, 1982.
8. J.G. Dick, Analytical Chemistry, Tata-McGraw Hill, 1973.
9. Alexis Leon and Mathews Leon, Fundamentals of Information Technology", Leon Vikas, Chennai, 1999.
10. Barbara Kasser, Using the Internet, 4thEdn., EE edition, New Delhi, 1998.
11. Sathyaprakash, Advanced Chemistry of Rar Elements, S. Chand & Col., 4thEdn., 1986.
12. T.Modlar, The chemistry of Lanthanides, Chapman and Hall, London, 1963.
13. H. D. Mathur and O.P. Tandon, Chemistry fo Rare Eleements, 3rdedn., S. Chand & Co., New Delhi, 1986.

Chemical kinetics, surface, biophysical and photochemistry

Programme: **M. Sc., Chemistry** Part: **Core-III**

Semester: **IV** Hours: *5*

Subject Code: **17PCHC43** Credits: 4

Course Outcomes

Elucidate rate of reactions, adsorption and chemical reactions by absorption of light radiations.

Unit I: Chemical kinetics I

Potential energy surfaces: Chain reactions-general characteristics- Steady state approximations-Study of kinetics of Chain reactions like H_2-Br_2 reaction-decomposition of N_2O_5 and acetaldehyde.

Unimolecular reaction rate theories-the simple Lindemann treatment-Hinshelwood's theory-Rice, Ramsperer and Kessel (RRK) theory-Advanced Unimolecular theory-Marcus theory or Rice, RamspererKessel and Marcus (RRKM) theory-Slater's theory. Principle of microscopic reversibility and detailed balancing-Reactions in solution- influence of solvent dielectric constant, ionic strength (Bronsted-Bjerrum equation)- Significance of volume of activation.

Unit II: Chemical kinetics II and catalysis

Fast reactions techniques-chemical relaxation methods, temperature and pressure jump methods, ultrasonic absorption techniques, reactions in flow system, continuous and stopped flow, shock wave tube methods., chemical kinetics in crossed molecular beams- Flash photolysis- Spin resonance techniques in study of reaction kinetics.

Catalysis in biological systems-Enzyme catalysis-Michaelis-Menton kinetics-Lineweaver and Burk plot-Eadie's plot-influence of pH on the Enzyme catalysis. Heterogeneous catalysis- chemical reactions on solid surfaces- Kinetics and mechanism of Unimolecular and bimolecular reaction- Langmuir, Hinshelwood's theory and Langmuir-Rideal mechanism-ARRT of surface reactions.

Unit III: Surface chemistry

Introduction-Adsorption of gases on solids-Physisorption and chemisorptions-adsorption isotherm- Freundlich- Langmuir-BET- Temkin adsorption isotherm- Adsorption on liquid surface-surface tension-Gibbs adsorption isotherm-surface area determination- Electro kinetic phenomena at interfaces including electro osmosis and electrophoresis- Spreading of a liquid on another surfactant-monolayers-preparation of LB films- Micelles- Critical micellar

concentration(CMC)-structure-bimolecular reaction occurring in a micellar solution-reverse micelles-micro emulsion- Application of photoelectron spectroscopy.

Unit IV: Biophysical chemistry

Basic concepts of non-equilibrium thermodynamics- Onsager reciprocal relationship- Its application to biological systems- High energy metabolites- ATP and its role in bioenergetics- transfer of potential and coupled reaction- Biological energy conversion in catabolism and anabolism- role of singlet oxygen in biology- Biophysical applications of Mossbauer effect- NMR imaging- Applications of spin labeling in membrane research- Molecular recognition – An introduction to supra-molecular chemistry and photochemistry.

Unit V: Photo and radiation chemistry

Photochemistry:

Photo physical processes in electronically excited molecules - Fluorescence, Phosphorescence and other deactivating processes. Stern-Volmerequationand its applications- electronically energy transfer mechanisms –photosensitization and chemiluminescence. Experimental techniques in photochemistry- light sources-chemical actinometry- Elementary aspects of photosynthesis, photochemical conversion and storage of solar energy.

Radiation chemistry:

Source of high energy- Interaction of high energy radiation with matter-Radiolysis of water- definition of G value- mode of reactions of hydrated electrons-OH^- and H^+. Experimental techniques of radiation chemistry- Dosimetry.

Books Recommended:

1. K.J.Laidler, Chemical kinetics,3rdEdn.,Harper International Edn,London(1987).
2. K.J.Laidler,Theories of Chemical Reaction Rates, McGraw Hill Book Co., London(1969).
3. F.Wilkinson, Chemical kinetics and Reaction mechanism, Van Nostrand Reinhold Co.,New York(1980).
4. C.Kalidas, Chemical kinetic Methods, New Age International, 1996.
5. Margaret Robson Wright, Fundamental Chemical kinetics-An Explanatory introduction to the concepts,Horwood Publishing Ltd.,West Sussex 1999
6. A.W.Adamson, Physical Chemistry of surfaces,5thEdn., John Wiley & Sons, New York(1990).
7. D.Attwood and A.T.Florence, Surfactant Systems- Their chemistry, Pharmacy and Biology, Chapman and Hall, New York (1983).
8. K.K. Rohatgi Mukherjee, Fundamentals of Photochemistry, Wiley Eastern.
9. N.J. Turro, Modern Molecular Photochemistry,Benjamin Cummings.
10. Hamil, Williams and Mackay, Pronciples of physical Chemistry II Edn.,Prentice-hall of India, Pvt., Ltd., New Delhi(1968). (Radiation Chemistry)

Semester IV

Project

17PCHC4P	Project – Viva– Voce	Hours 10/Credits 4

Course Outcomes

CO1: Formulate a research a topic

CO2: Familiar with the various stages of research process

CO3: Carried out projects in different fields of chemistry

Project titles will be allotted by the Research Guides (the Teachers in the Department) in areas related to the courses taught in the previous semester; they may also allot topics related to the other works apart from the prescribed text.

INTERNAL MARKS	40	MARKS
EXTERNAL EVALUATION (Viva – Voce)	60	MARKS
TOTAL	100	MARKS

Polymer chemistry

Programme: **M. Sc., Chemistry** Part: **Elective – I**

Semester: **IV** Hours: *5*

Subject Code: **17PCHE41** Credits: *5*

Course Outcomes

Characterize types of polymers, polymerization techniques and polymer processing.

Unit I: Classification of polymers and chemistry of polymerization

Classification of polymers: linear polymers, non-linear polymers, branched polymers, cross linked polymers, homo chains, hetero chains, homo polymers, co polymers, block polymers and graft polymers.

Chemistry of polymerization: Types of polymerization-mechanism-chain, growth, free radical, ionic, co-ordination, ring opening, metathetical, group transfer, polyaddition and polycondensation polymerizations.

Unit II: Individual polymers

Monomers required general methods of preparation, repeat Units and uses of the following polymers and resins- polyethylene, polystyrene, polyacrylonitrile, polymethymethacrylate, PVC, polytetrafluoroethylene, polyisoprenes, polybutadienes and polychloroprene, polyesters. Polycarbonates, polyimides, polyamides (Kevlar), polyurethanes, polyethyleneglycols, phenol-formaldehyde, urea-formaldehyde, melamine-formaldehyde and epoxy resins-silicone polymers.

Unit III: Properties of polymers

Intrinsic properties-processing properties-article properties-basic idea of isomerism of polymers-configuration of polymer chain-geometrical structure-syndiotatic, isotatic and atatic polymers

Glass transition temperature:

Definition-factors affecting glass transition temperature-relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticizer-importance of glass transition temperature- heat distortion temperature.

Molecular weight and size of polymers:

Number average, weight average, sedimentation and viscosity average molecular weights-molecular weights and degree of polymerization-poly dispersity-molecular weight distribution in polymers-size of polymer molecules- kinetics of polymerization.

Unit IV: Polymerization techniques, degradation and uses of polymers

Polymerization techniques:

Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation polymerizations.

Degradation:

Types of degradation - thermal, mechanical, ultrasonic and photodegradation photostabilizers - oxidative degradation – antioxidants - hydrolytic degradation.

Uses of polymers:

Electronics and biomedicine.

Unit V: Polymer processing

Plastics (thermo and thermosetting), elastomers, fibres, compounding, plasticisers, colorants, flame retardants. Compression and injection mouldings - film extrusion and calendaring - die casting and rotational casting - thermofoaming-reinforcing.

Books Recommended:

1. V.R. Gowariker, N.V. Viswanathan and JayadevSreedher, "Polymer Science", Wiley Eastern Ltd., New Delhi 1986.
2. G. Odian, "Principles of Polymerisation", 2nd edn., John Wiley and sons, New York, 1981.
3. D.W. van Krevelen and P.J. Hoftyrager, "Properties of Polymers", Elsevier, New York, 1976.
4. B.K. Sharma, "Polymer Chemistry", Goel Publishing House, Meerut, 1989.
5. P.J. Flory, "Principles of Polymer Chemistry", Cornell Univ. press, Ithaca, 1953.
6. F.W. Billmeyer, "Text Book of Poymer Science", 3rd edn., John Wiley and sons, New York, 1984.
7. Harry R. Allcock, F. W. Lampe and J.E. Mark, " Contemporary Polymer Chemistry", 3rd Edition, Pearson, Prentice Hall, New Delhi 2005.

Conducting Polymers

Programme: M. Sc., Chemistry Part: Elective – II

Semester: IV Hours: 5

Subject Code: 17PCHE42 Credits: 5

Course Outcomes

To understood basic concepts and synthetic methods, electrochemical synthesis, semiconducting and metallic polymers, doping and catalytic conducting polymers.

Unit: I Basic Concepts and Synthetic methods

Basics of conducting polymers - Organic - conjugated unsaturated hydrocarbons- Chemical Synthesis of conducting polymers – Other synthetic methods.

Unit: II Electrochemical Synthesis

Electrochemical synthesis of conducting polymers – monomers, electrolytic condition, electrodes and mechanism; Electrochemical synthesis of derivatives of poly pyrrole, polythiophene, polyazulene, polycarbazole, polyindole, polyaniline and polyphenylene.

Unit: III Semiconducting and Metallic Polymers

Structural basis for semiconducting and metallic polymers – introduction; Organic meta polymers - Synthetic route, isomers and electronic structure (polymers like polyacetylene, poly(p-phenylene), polypyrrole, polythiophene, etc.,).

Unit: IV Doping

Electrochemical doping; deadline to the development of conducting polymers; role of reduction and oxidation potential in doping; polyacetylene as electrode materials.

Unit: V Catalytic Conducting Polymers

Catalytic properties of conducting polymers; catalysis of electron donor-acceptor complexes; electrocatalysis by semiconducting polymers.

Books Recommended:

1. Terje A. Skotheim, Ronald L. Elsenbaumer, John R. Reynolds, Handbook of Conducting Polymers, Second Edition, Marcel Dekkar, 1995.
2. Hari Singh Nalwa (Edn), Handbook of Organic Conductive Molecules and Polymers, Four Volumes, Wiley, 1997
3. Jean-Pierre Farges, Organic Conductors, Marcel Dekkar, 1994
4. David B Cotts, Z Reyes, Electrically Conductive Organic Polymers for Advanced Applications, William Andrew Inc,1987
5. Larry Rupprecht, Conductive Polymers and Plastics, William Andrew Inc, 1999.
6. Raymond B Seymour, New Concepts in Polymer Science, Polymeric Composites, VSP, 1990.
7. Wallace Gordon, Gordon G Wallace, Geoffrey M Spinks, Conductive Electroactive Polymers, CRC Press, 2002.