

# DEPARTMENT OF CHEMISTRY

## M.Sc., (Chemistry)-SYLLABUS

Effect from the Academic Year 2016-2017



### MAHENDRA ARTS & SCIENCE COLLEGE (AUTONOMOUS)

['A' Grade Accredited by NAAC & Recognized under u/s 2(f) and 12B of the  
UGC act 1956]

**KALIPPATTI-637501**

**MAHENDRA ARTS & SCIENCE COLLEGE (AUTONOMOUS), KALLIPATTI**  
**M.Sc., CHEMISTRY Course structure for CBCS (2016-2017 onwards)**

SEM	Course Title	Sub Code	Hrs/ Week	Cred it	Ex Hr	Marks		Total
						IA	EA	
I	Organic Chemistry-I	M16PCH01	5	4	3	25	75	100
	Inorganic Chemistry-I	M16PCH02	5	4	3	25	75	100
	Physical Chemistry-I	M16PCH03	5	4	3	25	75	100
	Elective – I - Polymer Chemistry	M16PCHE01	6	4	3	25	75	100
	Value added - General Trends in Applied Chemistry (Seminar & Report)	M16PCHVA01	1	-	-	-	100	100
	Practical – I - Organic Chemistry - I	M16PCHP01	3	-	-	-	-	-
	Practical – II - Inorganic Chemistry - I	M16PCHP02	3	-	-	-	-	-
	Practical – III - Physical Chemistry – I	M16PCHP03	3	-	-	-	-	-
II	Organic Chemistry-II	M16PCH04	5	4	3	25	75	100
	Physical Chemistry-II	M16PCH05	5	4	3	25	75	100
	Elective – II - Coordination Chemistry	M16PCHE07	5	4	3	25	75	100
	Value added - General Trends in Applied Chemistry (Seminar & Report)	M16PCHVA01	2	2	-	-	100	100
	Practical – I - Organic Chemistry - I	M16PCHP01	3	4	6	40	60	100
	Practical – II - Inorganic Chemistry - I	M16PCHP02	3	4	6	40	60	100
	Practical – III - Physical Chemistry – I	M16PCHP03	3	4	6	40	60	100
	EDC – Fundamentals of computers and Communications	M16PCSED1	4	-	3	25	75	100
III	Human Rights	M16PHR01	-	2	3	-	100	100
	Organic Chemistry-III	M16PCH06	5	5	3	25	75	100
	Inorganic Chemistry-II	M16PCH07	5	5	3	25	75	100
	Physical Chemistry-III	M16PCH08	5	5	3	25	75	100
	Elective – III - Electrochemistry, Spectroscopy and Analytical Techniques	M16PCHE09	5	4	-	-	-	100
	Practical – IV - Organic Chemistry – II	M16PCHP04	3	-	-	-	-	-
	Practical – V- Inorganic Chemistry - II	M16PCHP05	3	-	-	-	-	-
	Practical – VI - Physical Chemistry - II	M16PCHP06	3	-	-	-	-	-
IV	Organic Chemistry - IV	M16PCH09	6	5	3	25	75	100
	Inorganic Chemistry-III	M16PCH10	6	5	3	25	75	100
	Practical – IV - Organic Chemistry – II	M16PCHP04	3	3	6	40	60	100
	Practical – V- Inorganic Chemistry - II	M16PCHP05	3	3	6	40	60	100
	Practical – VI - Physical Chemistry - II	M16PCHP06	3	3	6	40	60	100
	Project Report	M16PCHPR01	6	4	3	50	150	200
<b>Grand total</b>			<b>120</b>	<b>90</b>				

MAJOR	M.Sc. Chemistry	2016-2017
M16PCH01	<b>ORGANIC CHEMISTRY-I</b>	
Credits: 4		

### UNIT-I: STRUCTURE, REACTIVITY AND INTERMEDIATES

- 1.1 Resonance, field effects, hyperconjugation, steric effects, steric inhibition of resonance. Quantitative treatment of field and resonance effects – Hammett and Taft treatments-Acidity of carboxylic acids and phenols, basicity of aliphatic and aromatic bases.
- 1.2 Study and description of organic reaction mechanisms.
- 1.2.1 Non – kinetic methods – Energy profile diagrams, intermediate versus transition state, identification of products, Cross – over experiments, Stereochemical studies – uses of isotopes.
- 1.2.2 Kinetic methods: kinetic isotopic effects, salt effects, solvent effect, solvent isotopic effects, kinetic and thermodynamic controlled product. Hammond postulates. Curtin – Hammett principle.
- 1.3 Reactive intermediates: Generation, detection, stability and reactivity of Carbocations, carbanions, carbenes, arynes, nitrenes and free radicals, anions and cations.

### UNIT-II: STEREOCHEMISTRY

- 2.1 Interconversion of perspective, Fischer, sawhorse and Newman structures. Cram's and Prelog's rules; D, L, R, S-notations; Cahn-Ingold-Prelog rules, absolute and relative configurations; configurations of allenes, spiranes, biphenyls, cyclooctene, and helicene.
- 2.2 Conformation and reactivity in cyclohexane - Conformational analysis of disubstituted cyclohexanes and their stereochemical features - Conformation and reactivity of cyclohexanols (oxidation and acylation), cyclohexanones (reduction) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis). Conformation and stereochemistry of cis and trans decalins.
- 2.3 Geometrical and optical isomerism of disubstituted cyclopropane, cyclobutane and cyclopentanes. Identification of enantiotropic, homotropic, diastereotropic hydrogens and prochiral carbons – Stereospecific and stereoselective synthesis

### UNIT-III: AROMATIC ELECTROPHILIC AND NUCLEOPHILIC SUBSTITUTION

- 3.1 Aromaticity of non – benzenoid and hetrocyclic compounds – Aromatic electrophilic substitutions: Mechanism, orientation and reactivity – Quantitative treatment of reactivity in the substrate and reactivity of the electrophiles.
- 3.2 Electrophilic substitution: Mechanistic interpretations of second substitution, orientation and reactivity – the ortho/para ratio- ipso attack, third substitution, orientation and reactivity of other ring systems like polycyclic aromatic hydrocarbons, diazonium coupling, Vilsmeier reaction, Gattermann – Koch reaction.
- 3.3 Reactions involving a) Nitrogen electrophiles: nitration, nitrosation and diazonium coupling b) Sulphur electrophiles: sulphonation c) Halogen electrophiles: chlorination and bromination d) Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions.

3.4 Nucleophilic substitution:  $S_NAr$ ,  $S_N1$ , benzyne and  $SR_N1$  mechanisms-Reactivity – effect of substrate structure, leaving group and nucleophile. The Von Richter and Smiles rearrangements.

**Self study:** orientation and reactivities of 5 and 6 membered rings containing one and two hetero atoms in electrophilic substitutions and Nucleophilic substitutions.

#### **UNIT-IV: ALIPHATIC NUCLEOPHILIC SUBSTITUTION AND ELIMINATION REACTIONS**

4.1 Substitution at  $sp^3$  carbon atom –  $S_N1$  and  $S_N2$  mechanisms, ion pair in  $S_N1$ . Factors influencing  $S_N1$  and  $S_N2$  reactions – substrate, leaving group, nucleophile and solvent effects, ambident substrates and nucleophiles – regioselectivity. Border line cases: intermediate mechanism, Mixed  $S_N1$  and  $S_N2$  mechanisms. Neighboring group participation, non-classical carbocations.  $S_Ni$  mechanism, Allylic rearrangements.

4.2 Substitution at a trigonal carbon atom – the tetrahedral mechanism, formation of acid derivatives, cleavage of esters and N-acylation reactions. Substitution at vinyl carbon – tetrahedral and addition – elimination mechanisms.

4.3 Aliphatic substitution Mechanisms:  $S_E1$ ,  $S_E2$  and  $S_{Ei}$ ; Substitution by double bond shifts; other mechanism: addition – elimination and cyclic mechanism. Electrophilic substitution via enolization, Stork – enamine reaction.

#### **UNIT -V: ADDITION REACTIONS**

5.1 Elimination Reactions:  $E1$ ,  $E2$  and  $E1cB$  mechanisms, competition between elimination and substitution, orientation of product formation, stereochemistry of  $E2$  reactions, intermolecular pyrolytic eliminations, the Chugaev reaction, Cope elimination.

5.2 Addition reactions: Electrophilic addition to alkenes, mechanism, effect of structure, isotope effects, orientation and stereochemistry, the nature of the intermediates, Ozonolysis, hydroboration, additions to dienes, alkynes (halogenation and hydrogenation) and allenes, Diels-Alder reaction, 1,3 dipolar additions.

5.3 Nucleophilic addition to multiple bonds, Mannich reactions-Aldol and related reactions, Stobbe, Cannizzaro reaction, Darzens, Thorpe and Wittig reaction, benzoin condensation.

#### **TEXT BOOKS**

1. Advanced Organic Chemistry, Part A: Structure and Mechanisms, F. A. Carey and R. A. Sundberg, Fifth edition, Springer, New York, 2007.
2. Stereochemistry of Organic Compounds. Principles and Applications, D. Nasipuri, Second Edition, Wiley Eastern Limited, New Delhi, 1994. Ch.2-6 and 9-12.
3. J. March and M Smith, Advanced Organic Chemistry, 5<sup>th</sup> ed., John-Wiley and sons, 2001.
4. P. S. Kalsi, Stereochemistry of carbon compounds, 3rd edn, New Age International Publishers, 1995.

#### **REFERENCE BOOKS**

1. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata-McGraw Hill, 2000.

2. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd ed., New Age Publishers, 2005.
3. I. L. Finar, Organic Chemistry. Vol-2, 5th ed., Pearson Education Asia, 1975.
4. I. L. Finar, Organic chemistry, Vol-1, 6th ed., Pearson Education Asia, 2004.

MAJOR	M.Sc. Chemistry	2016-2017
M16PCH02	<b>INORGANIC CHEMISTRY-I</b>	
Credits: 4		

### **UNIT – I: ATOMIC STRUCTURE AND BONDING**

Atomic Structure and Periodic Table: Atom as nucleus with orbital electrons, concept of wave-functions, quantum numbers and spin, shape of s, p and d orbitals and their radial distribution functions, electronic configuration of atoms, Aufbau principle, Pauli Exclusion Principle, and Hund's rule; arrangement of elements in Groups in the Periodic Table, s-block, p-block, d-block and f-block elements; periodic properties, ionic radii, ionization potential, electron affinity, electronegativity (Pauling, Mulliken and Alfred-Rochnow scales); atomic states and term symbols.

Bonding and structure: Types of bonds, ionic, covalent, coordinate, double and triple bonds; orbital symmetry and overlaps, concept of MO and VB theory, concept of hybridization, the extent of d orbital participation in molecular bonding; bond energy and covalent radii, concept of resonance, bond moment and molecular dipole moment; polarizing power and polarizability, Fajan's rules.

### **UNIT – II: SOLID STATE AND NUCLEAR CHEMISTRY**

Inorganic Solids and Nuclear Chemistry: Types of solids, covalent, ionic, molecular and metallic solids, lattice energy, cohesive energy and Madelung constants, Van der Waals forces, hydrogen bonding, unit cell, crystal lattices, structure of simple ionic compounds, z radius ratio and closed packed structures. Imperfections in crystals (point defects and F centers).

Nuclear chemistry: nuclear reactions, Q value, cross sections, types of reactions, chemical effects of nuclear transformations; fission and fusion, fission products and fission yields; radioactive decay and equilibrium, radioactive techniques, tracer technique, neutron activation analysis, counting techniques such as G. M. ionisation and proportional counter.

### **UNIT – III: COMPOUNDS OF BORON AND SILICON**

Synthesis, properties and structures of Boron and Silicon compounds: Boron hydrides (small boranes and their anions, B1–B4), boron nitride, borazines, carboranes, metalloboranes, metallocarboranes; silicates, silicones, diamond, graphite, zeolites.

### **UNIT – IV: COMPOUNDS OF SULFUR, NITROGEN, PHOSPHOROUS AND NOBEL GAS**

Nitrogen, Phosphorous, Sulphur and noble gas compounds: Hydrides, oxides and oxy acids of Nitrogen, Phosphorous, Sulphur and halogens; phosphazines, sulphur-nitrogen compounds, inter halogen compounds, pseudo halogens, noble gas compounds.

## UNIT – V: POLYANIONS AND CLATHRATES

Poly anions and isopoly anions of Phosphorous, Vanadium, Chromium, Molybdenum and Tungsten, heteropoly anions of Molybdenum and Tungsten; clathrates (noble gases, phosphazines) hydrogen bonding in clathrates, Phosphorous and Oxygen cage compounds.

### RECOMMENDED BOOKS:

1. J. E. Huheey, Inorganic Chemistry, Principles, Structure and Reactivity, Harper and Row, 3rd Edn, 1983.
2. D. F. Shriver, P.W. Atkins, C.H. Langford, Inorganic Chemistry, 2nd Edn, ELBS, 1994.
3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, A comprehensive Text, John Wiley, 5th Edn, 1987.
4. H. J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 2nd Edn, 1988.
5. C. N. R. Rao and J.Gopalakrishnan, New Directions in Solid State Chemistry.
6. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, 2001.
7. J. D. Lee, A New Concise Inorganic Chemistry, 3rd Edn., ELBS, 1987.

MAJOR	M.Sc. Chemistry	2016-2017
M16PCH03	<b>PHYSICAL CHEMISTRY-I</b>	
Credits: 4		

### **UNIT – I: CLASSICAL THERMODYNAMICS – I**

Maxwell's relations and thermodynamic equations of state – applications in the evaluation of  $C_p - C_v$  for solids and for vanderwaals gases,  $C_p - C_v$  in terms of coefficient of expansion and coefficient of compressibility – Relation between  $C_p$  and  $C_v$  – Partial molar properties – Gibbs – Duhem equation – Partial molar free energy (Chemical Potential) – Determination of chemical potential [Direct Method and Method of Intercepts] and partial molar volume – variation of chemical potential with Temperature and Pressure

### **UNIT – II: CHEMICAL KINETICS – I**

Theories of Reaction rates – Arrhenius theory – effect of temperature on reaction rate – Hard – Sphere collision theory of reaction rates – molecular beams – Reaction cross section – effectiveness of collisions – Probability factor.

Transition state theory of reaction rates – Potential energy surface – Partition functions and activated complex – Eyring equation – Comparison of collision theory and activated complex theory – Estimation of free energy, enthalpy and entropy of activation and their significance.

### **UNIT – III: QUANTUM CHEMISTRY – I**

Black body Radiation – Experimental results of Black body radiation – Photoelectric effect – De – Broglie equation – Heisenberg uncertainty principle – Compton effect – operators and commutation relations – quantum mechanical postulates – Schrodinger equation and its solution to the problem of a particle in one and three dimensional boxes – the harmonic oscillator.

### **UNIT – IV: GROUP THEORY – I**

Symmetry elements and symmetry operations – Point groups – identification and representation of groups – comparison of Molecular symmetry with Crystallographic symmetry – Reducible and irreducible representation – Direct product representation – Great orthogonality theorem and its consequences – Character Table and their uses.

### **UNIT – V: SPECTROSCOPY – I**

Interaction of matter with radiation– Rotation spectroscopy – Rigid Rotor – Intensity of spectral lines – Molecular parameters from rotation spectra - Effect of isotopic substitution on the rotation spectra. Vibrational spectroscopy – harmonic oscillator – anharmonic oscillator – Hot bands – selection rules – Vibrational spectra of polyatomic molecules – Overtones and combination frequencies – Fermi Resonance.



Raman spectroscopy – Raman effect – Rotational and vibrational Raman Spectra – Mutual Exclusion Rule. Electronic spectroscopy – Electronic spectra of diatomic molecules – vibrational coarse structure – Franck – Condon Principle.

### **TEXT BOOKS:**

1. S.Glasstone, Thermodynamics for chemists, Affiliated East West press, New Delhi, 1960.
2. J. Rajaram and J.C. Kuriacose, Thermodynamics for students of chemistry, Lal Nagin Chand, New Delhi, 1986.
3. J. Rajaram and J.C. Kuriacose, Kinetics and mechanism of chemical transformation Macmillan India Ltd., 1993.
4. K.J.Laidlar, Chemical Kinetics, Harper and Row Newyork, 1987.
5. D.A. Mcquarrie, Quantum chemistry, University science books, Mill Valley, California (1983)
6. .K. Prasad, Quantum Chemistry, Wiley Eastern, New Delhi, 1992.
7. V.Ramakrishnan and M.S.Gopinathan, Group theory in chemistry, Vishal Publications, 1988.
8. V.Raman, Group theory and its application to chemistry, Tata McGraw Hill Publishing Co., 1990.
9. Raymond chang, Basic principles of Spectroscopy, McGraw Hill Ltd., New York, 1971.
10. C.N. Banwell, Fundamentals of Molecular Spectroscopy, Mc Graw Hill, Newyork 1966.

### **REFERENCE BOOKS:**

1. W.J. Moore, Physical Chemistry, Orient Longman, London, 1972.
2. K.G. Den beigh, Thermodynamics of Steady state, Meklien and Co., London, 1951.
3. L. K. Nash, Elements of Chemical Thermodynamics, Addison Wesley, 1962.
4. R. G.Frost and Pearson, Kinetics and Mechanism, Wiley, Newyork, 1961.
5. W. Moore and R.G. Pearson, Kinetics and Mechanism, 1981.
6. C.Capellos and B.H.J. Bielski, Kinetic systems, Willey interscience, Newyork, 1968.
7. G. M.Harris, Chemical Kinetics, D.C. Heath and Co., 1966.
8. I. N.Levine, Quantum chemistry, Allyn and Bacon, Boston, 1983.
9. J. Goodman, Contemporary Quantum Chemistry, An Introduction, Plenum Press, Newyork, 1977.
10. F.J.Bockhoff, Elements of Quantum theory, Addison Wesley, Reading, Mass, 1976.
11. P.W.Atkins, Physical Chemistry, Oxford University Press, Oxford., 1990.
12. P.W.Atkins, Molecular Quantum Mechanics, Oxford University Press, Oxford., 1983.
13. H.Eyring, J.Walter and G. Kimball, Quantum chemistry, John wiley and sons, Newyork, 1944.
14. L.S.Pauling and E.B.Wilsob, Introduction to Quantum Mechanics, Mc Graw Hill book Co., Newyork, 1935.
15. F.A. Cotton, Chemical Application of Group Theory, John wiley and Sons Inc., Newyork, 1971.

16. N. Tinkham, Group Theory and Quantum Mechanics, McGraw Hill Book Company, Newyork, 1964.
17. Alan Vincent, Molecular Symmetry and Group theory – Programmed Introduction to chemical applications, Wiley, Newyork, 1977.
18. G.M. Barrow, Introduction to Molecular Spectroscopy, Mc Grawhill, Newyork, 1962.
19. G.W.King, Spectroscopy and Molecular Structure, Holt, Rienehart and Winston, 1964.
20. E.B.Wilson, J.C. Decius and D.C.Cross, Molecular Vibrations, Mc Graw Hill Book Co., 1955.
21. B.P. Straughan and S.Walker, Spectroscopy Vol-I, Vol-II and Vol-III, Chapmann and Hall, 1976.

ELECTIVE-I	M.Sc. Chemistry	2016-2017
M16PCHE01	<b>POLYMER CHEMISTRY</b>	
Credits: 4		

### **UNIT – I: BASIC CONCEPTS**

Monomers, repeat units, degree of polymerization, Linear, branched and network Polymers. Condensation Polymerization : Mechanism of stepwise polymerization. Kinetics and statistics of linear stepwise polymerization. Addition polymerization : Free radical, cationic and anionic polymerization. Polymerization conditions. Polymerization in homogeneous and heterogeneous systems.

### **UNIT – II: CO-ORDINATION POLYMERIZATION**

Kinetics, mono and bimetallic mechanism of co-ordination polymers. Zeigler Natta catalyst, co-polymerization: Block and graft co-polymers, kinetics of copolymerization. Types of co-polymerization. Reactivity ratio.

### **UNIT – III: MOLECULAR WEIGHT AND PROPERTIES**

Polydispersion – average molecular weight concept, number, weight and viscosity average molecular weights. Measurement of molecular weights. Viscosity, light scattering, osmotic and ultracentrifugation methods. Polymer structure and physical properties – crystalline melting point  $T_m$ . The glass transition temperature. Determination of  $T_g$ . Relationship between  $T_m$  and  $T_g$ .

### **UNIT – IV: POLYMER PROCESSING**

Plastics, elastomers and fibres. Compounding, processing techniques: calendering, die casting, rotational casting, film casting, injection moulding, blow moulding extrusion, moulding, thermoforming, foaming, reinforcing and fibre spinning.

### **UNIT – V: PROPERTIES OF COMMERCIAL POLYMERS**

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers, Fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

#### **Text Books**

1. F.W. Billmeyer, TextBook of Polymer Science, 3rd Edition, J.Wiley, 2003.
2. Gowariker, N.V. Viswanathan and J. Sreedhar, Polymer Science, New Age Int., 1986.

#### **Reference Books**

1. H.R. Alcock and F.W. Lamber, Contemporary Polymer Chemistry, Prentice Hall, 1981.
2. P.J. Flory, Principles of Polymer Chemistry, Cornell University press, New York, 1953.
3. G. Odian, Principles of Polymerization, 2nd Edition, John Wiley & Sons, New York, 1981

ELECTIVE-I	M.Sc. Chemistry	2016-2017
M16PCHE02	<b>APPLIED ELECTROCHEMISTRY</b>	
Credits: 4		

### **UNIT – I: INTRODUCTION**

Overview of electrochemical concepts and methods; the electrochemical experiment; electrochemical methods; sign conventions; the three-electrode cell, the potentiostat, electrochemical window, types of electrodes.

### **UNIT –II: THERMODYNAMICS**

Redox reactions; cell notation; standard potentials, free energy & equilibrium constants; the SHE; the Nernst equation; activity and formal potentials; reference electrodes, etc.

### **UNIT –III: THE ELECTRIFIED INTERFACE**

Electric double layer; Helmholtz and Gouy-Chapman models; the dropping mercury electrode; surface tension; double-layer capacitance; specific and non-specific adsorption; Debye-Hückel theory, etc.

### **UNIT –IV: ELECTRON TRANSFER KINETICS**

Standard rate constant; transfer coefficient; Tafel equation; Marcus theory; Butler-Volmer equation; Tafel plots; irreversible & quasi-reversible voltammetry, etc.

### **UNIT –V: POTENTIOMETRY**

Two types; general methods and calibration; redox and ion-selective electrodes, etc.

### **REFERENCE BOOKS**

1. Encyclopedia of Applied Electrochemistry ISBN: 978-1-4419-6995-8.
2. Electro analysis theory and applications in aqueous and non-aqueous media and in automated chemical control, E.A.M. F. Dahmen, 1986.

ELECTIVE-I	M.Sc. Chemistry	2016-2017
M16PCHE03	<b>GREEN CHEMISTRY</b>	
Credits: 4		

### UNIT-I: GREEN CHEMISTRY

Introduction to green chemistry: Green chemistry-relevance and goals, Anastas' twelve principles of green chemistry - Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

### UNIT-II: MICROWAVE MEDIATED ORGANIC SYNTHESIS (MAOS)

Microwave activation – advantage of microwave exposure – specific effects of microwave – Neat reactions – solid supports reactions – Functional group transformations – condensations reactions – oxidations – reductions reactions – multi-component reactions.

### UNIT-III: IONIC LIQUIDS

Ionic liquids and PTC Introduction – synthesis of ionic liquids – physical properties – applications in alkylation – hydroformylations – epoxidations – synthesis of ethers – Friedel-Craft reactions – Diels-Alder reactions – Knoevenagel condensations – Wittig reactions – Phase transfer catalyst - Synthesis – applications.

### UNIT-IV: BIO-CATALYSTS

Supported catalysts and bio-catalysts for Green chemistry Introduction – the concept of atom economy – supported metal catalysts – mesoporous silicas – the use of Biocatalysts for green chemistry.

### UNIT-V: MODIFIED BIO CATALYSTS

Fermentations and biotransformations – fine chemicals by microbial fermentations – vitamins and amino acids – Baker's yeast mediated biotransformations – Bio-catalyst mediated Baeyer-Villiger reactions – Microbial polyester synthesis.

### REFERENCE BOOKS

1. Green Chemistry – Environmentally benign reactions – V. K. Ahluwalia. Ane Books India (Publisher). (2006). Green Chemistry – Designing Chemistry for the Environment – edited by Paul T. Anastas & Tracy C. Williamson. Second Edition, (1998).
2. Green Chemistry – Frontiers in benign chemical synthesis and processes- edited by Paul T. Anastas & Tracy C. Williamson. Oxford University Press, (1998).
3. Green Chemistry – Environment friendly alternatives- edited by Rashmi Sanghi & M. M. Srivastava, Narora Publishing House, (2003).

ELECTIVE-I	M.Sc. Chemistry	2016-2017
M16PCHE04	<b>MATERIAL SCIENCE</b>	
Credits: 4		

### **UNIT-I: ADVANCED MATERIALS AND TOOLS**

Smart materials, exhibiting ferroelectric, piezoelectric, optoelectric, semiconducting behavior, lasers and optical fibers, photoconductivity and superconductivity, nanomaterials, synthesis, properties and applications, biomaterials, superalloys, shape memory alloys.

### **UNIT-II: MATERIALS CHARACTERIZATION TECHNIQUES**

Scanning electron microscopy, transmission electron microscopy, atomic force microscopy, scanning tunneling microscopy, atomic absorption spectroscopy, differential scanning calorimetry.

### **UNIT-III: MECHANICAL PROPERTIES**

Stress-strain diagrams of metallic, ceramic and polymeric materials, modulus of elasticity, yield strength, tensile strength, toughness, elongation, plastic deformation, viscoelasticity, hardness, impact strength, creep, fatigue, ductile and brittle fracture.

### **UNIT-IV: THERMAL PROPERTIES**

Heat capacity, thermal conductivity, thermal expansion of materials. Electronic Properties: Concept of energy band diagram for materials - conductors, semiconductors and insulators, electrical conductivity effect of temperature on conductivity, intrinsic and extrinsic semiconductors, dielectric properties.

### **UNIT-V: OPTICAL PROPERTIES**

Reflection, refraction, absorption and transmission of electromagnetic radiation in solids. Magnetic Properties: Origin of magnetism in metallic and ceramic materials, paramagnetism, diamagnetism, antiferro magnetism, ferromagnetism, ferrimagnetism, magnetic hysteresis.

### **REFERENCE BOOKS**

1. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, 2, Wiley – VCH, Weinheim, 2004.
2. C.P. Poole, Jr: F.J. Owens, Introduction to Nanotechnology Wiley Interscience, New Jersey, 2003 Kenneth J. Klabunde (Ed), Nanoscale materials in Chemistry, Wiley-Interscience, New York, 2001. T. Pradeep, Nano: The Essentials in understanding nanoscience and nanotechnology, Tata McGraw Hill, New Delhi, 2007.

MAJOR	M.Sc. Chemistry	2016-2017
M16PCH04	<b>ORGANIC CHEMISTRY-II</b>	
Credits: 4		

### **UNIT-I: UV AND VISIBLE SPECTROSCOPY AND IR**

Terminology, classification of electronic transitions. Effect of substituent and conjugation on the spectra of alkenes. Woodward – Fieser rules for polyenes. Electronic spectra of carbonyl compounds. Effect of solvent on  $\pi - \pi^*$  and  $n - \pi^*$  transitions. Woodward's rules for enones. Electronic spectra of benzene and its derivatives.

#### **IR spectroscopy**

Theory and principle, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides). Effect of solvent and hydrogen bonding on the vibrational frequencies in alcohols.

### **UNIT-II: NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY**

Introduction- Nuclear spin and nuclear parameters-NMR nuclei-Nuclear spin states. The mechanism of absorption( resonance condition).Calculation of resonance frequency. Population densities of nuclear spin states. Relaxation processes.

The chemical shift and shielding. Chemical environment and chemical shift. Factors affecting chemical shift. Magnetic anisotropy. Continuous wave and pulsed Fourier methods of recording NMR spectra. Spin – spin coupling and splitting of NMR signals. Spin – spin interactions – AX, AX<sub>2</sub>, AX<sub>3</sub>, AMX and AB types. The coupling constant. Intensities of multiplets – Pascal's triangle

Geminal and vicinal coupling. Karplus equation and Karplus curve. First and second order coupling of AB systems. Spin decoupling methods. Double resonance. Applications in structural elucidation.

### **UNIT-III: CARBON-13 NMR SPECTROSCOPY**

The carbon – 13 nucleus, carbon – 13 chemical shift. Proton coupled and proton decoupled carbon – 13 spectra. Nuclear overhauser effect. Problems with integration in carbon - 13 spectra. Off resonance decoupling. Applications. Introduction to <sup>19</sup>F, <sup>31</sup>P NMR spectra

### **UNIT-IV: ADVANCED NMR TECHNIQUES AND PROBLEMS**

Pulse sequences, spins and magnetization vectors. The DEPT experiment. Determining the number of attached hydrogens. Introduction to two – dimensional spectroscopic methods. The COSY technique. An overview of the COSY Experiment.

Problem solving exercises involving UV, IR NMR & MS data

## UNIT-V: MASS SPECTROSCOPY

Introduction, principle and instrumentation. Ion production – electron impact, chemical ionization, field desorption and fast atom bombardment techniques. High resolution mass spectrometry – base -, molecular ion -, parent ion -, fragmentation ion -, metastable – and isotopic peaks. Factors affecting fragmentation, ion analysis and ion abundance. Mass spectral fragmentation of organic compounds (hydrocarbons, aromatic compounds, alcohols, carbonyl compounds, acids and esters). McLafferty rearrangement. Determination of molecular weight and molecular formula.

### REFERENCE BOOKS

1. Physical methods in Inorganic chemistry, R.S. Drago, Affiliated East-West Press Pvt. Ltd., New Delhi (1965).
2. Infrared Spectra of Inorganic and co-ordination Compounds, K. Nakamoto, Wiley-Interscience, New York, (1970).
3. Vibrational spectroscopy: theory and Applications, D.N.Sathyanarayana, New-Age International Publishers, New Delhi (2000).
4. Electronic Absorption Spectroscopy and related techniques, D.N.Sathyanarayana, Universities Press, Bangalore, (2001).
5. Applications of absorption Spectroscopy to Organic Compounds, J.R. Dyer, Prentice – Hall, New Delhi, (1969).
6. Organic Spectroscopy, W. Kemp, ELBS London, (1975).
7. Spectrometric Identification of Organic Compounds, R.M. Silverstein and W.P. Webster, Wiley & Sons, (1999).
8. Organic Mass Spectroscopy, K.R. Dass and E.P. James, IBH New Delhi, (1976).
9. Principles of Instrumental Analysis, D.A. Skoog, S.J. Holler, T.A. Nilman, 5th Edition, Saunders College Publishing, London, (1998).
10. Introduction To Spectroscopy, 2nd Edition, Donald L. Pavia, Gary M. Lampman and George S. Keiz, Harcourt Brace College Publishers, (1996).
11. Physical Methods for Chemists, R.S. Drago, 2nd Edition, Saunders College Publishing New York, (1992).
12. Mass Spectrometry – Analytical Chemistry By Open Learning -, R. Davies, M. Frearson and E. Prichard, John Wiley and Sons, New York, (1987).



MAJOR	M.Sc. Chemistry	2016-2017
M16PCH05	<b>PHYSICAL CHEMISTRY-II</b>	
Credits: 4		

### **UNIT – I: CLASSICAL THERMODYNAMICS – II**

Thermodynamics of ideal and real gases, gas mixtures – Fugacity – definition – Methods of determination of fugacity – Variation of fugacity with temperature and pressure.

Standard states for gases, liquids, solids and components of solutions –determination of activities and activity coefficient from Vapour pressure, Freezing point, Boiling point and EMF – measurements.

Solution of Electrolytes – mean ionic activity, mean ionic molality and mean ionic activity coefficients – determination of activity coefficient from Freezing Point, EMF and Solubility measurements – Concept of ionic strength.

### **UNIT – II: CHEMICAL KINETICS – II**

Reactions in solutions – comparison between gas phase and solution reactions – the influence of solvent, ionic strength, dielectric constant and pressure on reaction in solution – Kinetic isotope effects – Linear free energy relationship – Hammett and Taft equations.

### **UNIT – III: QUANTUM CHEMISTRY –II**

Schrödinger equation for the rigid rotator and Hydrogen atom – arriving solution for energy and wave function – the origin of quantum numbers and their physical significance – Probability distribution of electrons.

Approximation methods – Perturbation and Variation methods – application of Variation method to Hydrogen and Helium atom – Spin - orbit interaction – LS coupling and JJ coupling – Term symbols and spectroscopic states. Ground state term symbols for simple atoms.

### **UNIT – IV: GROUP THEORY – II**

Symmetry selection rules for vibrational, Electronic and Raman Spectra – determination of representation of vibrational modes in non-linear molecules such as H<sub>2</sub>O, CH<sub>4</sub>, XeF<sub>4</sub>, SF<sub>6</sub> and NH<sub>3</sub> – symmetry of Hybrid orbitals in non-linear molecule (BF<sub>3</sub>, CH<sub>4</sub>, XeF<sub>4</sub>, PCl<sub>5</sub> and SF<sub>6</sub>) – Electronic spectra of formaldehyde.

### **UNIT – V: SURFACE CHEMISTRY AND CATALYSIS**

Kinetics of surface reactions: Physical and chemical adsorption – adsorption isotherms – types of adsorption isotherms – Langmuir adsorption isotherm – B.E.T theory for multilayer adsorption – measurement of surface area – Mechanism of heterogeneous catalytic reactions – the adsorption coefficient and its significance.

Acid – Base catalysis – mechanism – Bronsted catalysis Law – catalysis by enzymes – rate of enzyme catalysed reactions – effect of substrate concentration, pH and temperature on enzyme catalysed reactions – Michael – Menton's equation.

#### **TEXT BOOKS:**

1. S.Glasstone, Thermodynamics for chemists, Affiliated East West press, New Delhi, 1960.
2. J. Rajaram and J.C. Kuriacose, Thermodynamics for students of chemistry, Lal Nagin Chand, New Delhi, 1986.
3. J. Rajaram and J.C. Kuriacose, Kinetics and mechanism of chemical transformation, Macmillan India Ltd., 1993.
4. K.J.Laidlar, Chemical Kinetics, Harper and Row, Newyork, 1987.
5. R.K. Prasad, Quantum Chemistry, Wiley Eastern, New Delhi, 1992.
6. M.W. Hanna, Quantum mechanics in chemistry, W.A. Benjamin INC, London (1965)
7. V.Ramakrishnan and M.S.Gopinathan, Group theory in chemistry, Vishal Publications, 1988.
8. K.V.Raman, Group theory and its application to chemistry, Tata McGraw Hill Publishing Co., 1990.
9. Gurudeep raj, Advanced Physical Chemistry, Goel Publishing House, Meerut.

#### **REFERENCE BOOKS:**

1. W.J. Moore, Physical Chemistry, Orient Longman, London, 1972.
2. K.G. Den beigh, Thermodynamics of Steady state, Meklien and Co., London, 1951.
3. L.K. Nash, Elements of Chemical Thermodynamics, Addison Wesley, 1962.
4. R.G.Frost and Pearson, Kinetics and Mechanism, Wiley, Newyork, 1961.
5. J.W. Moore and R.G. Pearson, Kinetics and Mechanism, 1981.
6. C.Capellos and B.H.J. Bielski, Kinetic systems, Willey interscience, Newyork, 1968.
7. G.M.Harris, Chemical Kinetics, D.C. Heath and Co., 1966.
8. A.K. Chandra, Introductory Quantum Chemistry, Tata Mc Graw Hill.
9. D.A. Mc Quarrie, Quantum Chemistry, University science books, Mill Valley, California (1983).
10. P.W.Atkins, Molecular Quantum Mechanics, Oxford University Press, Oxford., 1983.
11. I.N.Levine, Quantum chemistry, Allyn and Bacon, Boston, 1983.
12. F.J.Bockhoff, Elements of Quantum theory, Addison Wesley, Reading, Mass, 1976.
13. H.Eyring, J.Walter and G. Kimball, Quantum chemistry, John wiley and sons, Newyork, 1944.
14. L.S.Pauling and E.B.Wilsob, Introduction to Quantum Mechanics, Mc Graw Hill book Co., Newyork, 1935.
15. F.A. Cotton, Chemical Application of Group Theory, John wiley and Sons Inc., Newyork, 1971.
16. N. Tinkham, Group Theory and Quantum Mechanics, McGraw Hill Book Company, Newyork, 1964.
17. Alan Vincent, Molecular Symmetry and Group theory – Programmed Introduction to chemical applications, Wiley, Newyork, 1977.

ELECTIVE-II	M.Sc. Chemistry	2016-2017
M16PCHE05	<b>PHYSICAL ORGANIC CHEMISTRY</b>	
Credits: 4		

### **UNIT- I: MODERN THEORY OF ORGANIC STRUCTURES AND BONDING**

Modern theory of organic structures and bonding. Symmetry-adapted orbitals. Perturbation theory and orbital mixing rules. Buildup approach to large molecular structures. Bonding and structure of reactive intermediates: Carbocations, carbanions, and carbenes. Relation between structure and energetics.

### **UNIT-II: SOLUTIONS**

Solutions and forces of molecular recognition. Bronsted acid-base chemistry. Lewis acids/bases, electrophiles and nucleophiles. Reactivity, kinetics, and mechanisms. Energy surfaces and transition states. Hammond Postulate.

### **UNIT-III: ISOTOPE EFFECTS**

Isotope effects. Hammett plot. Steric and polar effects. Empirical scales of solvent effect. pH and Bronsted relationship.

### **UNIT-IV: MECHANISM AND CATALYSIS**

Mechanism and catalysis of proton transfer. General principles of catalysis. Enzyme-catalytic effect and concept of transition-state stabilization.

### **UNIT-V: PHYSICAL ORGANIC APPROACH**

Investigation of organic reaction mechanisms by physical organic approach. Examples illustrating application to investigation of electrophilic/nucleophilic reactions, and enzyme-catalyzed reactions.

### **REFERENCE BOOKS:**

1. E. V. Anslyn and D. A. Dougherty, Modern Organic Chemistry, University Science, 2005. A. Pross, Theory and Physical Principles of Organic Reactivity, John Wiley, 1995.
2. A. Rauk, Orbital Interaction Theory of Organic Chemistry, John Wiley, 1994. T. H. Lowry and K. H. Richardson, Mechanisms and Theory in Organic Chemistry, Harper and Row, 1976.

ELECTIVE-II	M.Sc. Chemistry	2016-2017
M16PCHE06	<b>BIOORGANIC &amp; MEDICINAL CHEMISTRY</b>	
Credits: 4		

### **UNIT-I: AMINO ACIDS AND PROTEINS STRUCTURE**

Classification, synthesis and properties of amino acids, isoelectric point, biosynthesis of amino acids. Peptides: oligo- and polypeptides, geometry of peptide linkage, N-terminal and C-terminal residue analysis, synthesis of peptides-amino and carboxyl protecting groups-solid phase peptide synthesis. Proteins: classification and properties (denaturation, isoelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins, collagen and triple helix.

### **UNIT-II: ENZYMES AND COFACTORS**

Mechanism of enzyme catalysis, Factors influencing enzyme action, Examples of typical enzyme mechanisms: chymotrypsin, ribonuclease and lysozyme, Enzyme-catalyzed addition, elimination, condensation, carboxylation and decarboxylation, isomerisation, group transfer and rearrangement reactions-structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, lipoic acid and Vitamin B12. Mechanisms of reactions catalysed by the above cofactors.

### **UNIT-III: NUCLEIC ACIDS AND PROTEIN SYNTHESIS**

Nucleotides and nucleosides, DNA: primary and secondary structure-replication of DNA. RNA and protein synthesis: Messenger RNA synthesis-transcription, Ribosomes-rRNA, Transfer RNA, genetic code-translation. Determination of base sequence of DNA. Polymerase Chain Reaction (PCR). Antisense technology in chemotherapy and other nucleic acid-targeted drugs-intercalators, sequence specific drugs. A brief account of ribosome and iRNA.

### **UNIT-IV: LEAD AND ANALOGUE SYNTHESIS**

Designing organic synthesis-disconnection approach-synthons and synthetic equivalents-one group disconnections: alcohol, olefin, ketone, acids-two group disconnections: 1,2-, 1,3-, 1,4- and 1,5-difunctional compounds-convergent synthesis-functional group interconversions-functional group additions-carbonheteroatom bonds-methods for 3- to 6-membered rings. 17

### **UNIT-V: MEDICINAL CHEMISTRY**

Lead and Analogue Synthesis-2 Combinatorial synthesis in medicinal chemistry: Solid phase techniques-methods of parallel synthesis-mix and split techniques-dynamic combinatorial chemistry-screening and deconvolution-limitations of combinatorial synthesis Asymmetric synthesis: basic principles-stereoselective and stereospecific reactions- methods for determining enantiomeric excess-chiral auxiliary, reagents and catalysts and their applications (wherever applicable) in alkylation, hydrogenation, hydroxylation, epoxidation and hydroboration of

alkenes, reduction of ketones-Cram and Felkin-ahn models. Noyori's BINAP – Jacobson catalyst – Evans catalyst.

#### REFERENCE BOOKS:

1. Bioorganic Chemistry: A Chemical approach to Enzyme action, Hermann Dugas and C.Penny, Springer-Verlag.
2. Fundamentals of Enzymology, N.C. Price and L.Stevens, Oxford University Press.
3. Enzymatic Reaction Mechanisms, C. Walsh, W.H.Freeman.
4. Designing Organic Synthesis: The Disconnection Approach by Stuart Warren, Wiley, 2nd edition, 1984.
5. Asymmetric Synthesis by H. B. Kagan, Thieme Medical Publishers, 2003.
6. Advanced Organic Chemistry: Part-A and Part-B by Francis A. Carey and Richard B. Sundberg, Springer, 5th edition, 2007.

ELECTIVE-II	M.Sc. Chemistry	2016-2017
M16PCHE07	<b>COORDINATION CHEMISTRY</b>	
Credits: 4		

### **UNIT – I: Introduction to Transition Metal Complexes:**

Brief review of the general characteristics of transition elements, types of ligands, nomenclature of coordination complexes, chelates, chelate effect, geometry and isomerism, formation of complexes, stability constants, Werner, Sidzwick and VSEPR theory.

### **UNIT – II: Electronic Structure of Transition Metal Complexes 1:**

Crystal field theory, crystal field splitting, application of d-orbital splittings to explain magnetic properties, low spin and high spin complexes, crystal field stabilization energy, spectrochemical series, weak and strong field complexes, thermodynamic and related aspects of crystal fields, ionic radii, heats of ligation, lattice energies, site preference energies.

### **UNIT – III: Electronic Structure of Transition Metal Complexes 2:**

VB and MO theory of complexes (quantitative principles involved in complexes with no pi and with pi bonding) and ligand field theories and molecular symmetry, angular overlap model, Jahn Teller effect, electronic spectra of transition metal complexes, Term states of  $d^n$  ions, Orgal and Tanabe-Sugano diagrams, charge transfer and d-d transitions, nephelauxetic series.

### **UNIT – IV: Inorganic Reaction Mechanisms**

Inorganic reaction mechanisms: inert and labile compounds, substitution reactions of octahedral complexes, dissociative, associative, anation, aquation, conjugate base mechanism; substitution reactions of square planar complexes, trans effect, trans effect series, theories of trans effect; electron transfer reactions.

### **UNIT – V: Inorganic Clusters**

Inorganic chains - rings - cages and clusters - catenation - heterocatenation - intercalation chemistry - one dimensional conductor - isopolyanions - heteropolyanions - borazines - phosphazenes - phosphazene polymers - ring compounds of sulphur and nitrogen - homocyclic inorganic systems - cages - boron cage compounds - metal clusters - dinuclear clusters - trinuclear clusters - tetranuclear clusters - hexanuclear clusters - structural prediction of organometallic clusters.

### **RECOMMENDED BOOKS:**

1. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.
2. J. E. Huheey, Inorganic Chemistry, 3rd Edn., Harper International, 1983.
3. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, 2001.
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.
5. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., BH, 1997.
6. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.
7. J. D. Lee, A New Concise Inorganic Chemistry, 3rd Edn., ELBS, 1987.

ELECTIVE-II	M.Sc. Chemistry	2016-2017
M16PCHE08	<b>SCIENTIFIC RESEARCH METHODOLOGY</b>	
Credits: 4		

### **UNIT – I: INTRODUCTION**

Introduction to Research Methodology Research Problem and Research Design Formulation of Hypotheses.

### **UNIT – II: RESEARCH METHODS**

Types of Research Methods: Quantitative and Qualitative Research Techniques and Tools.

### **UNIT – III: RECORDS**

Questionnaire, Interview, Observation, Schedule, Check-list, Library Records and Reports. Metric Studies in LIS

### **UNIT – IV: DATA ANALYSIS**

Data Analysis and Interpretation Data Analysis: Statistical Methods Data Analysis : Computer Processing Interpretation and Presentation of Results

### **UNIT –V: REPORTS**

Report Writing Research- Report Writing Style Manuals IPR and Plagiarism.

### **REFERENCE BOOKS:**

1. Connaway (L S) & Powell (R R). Basic research methods for librarians (Ed.5), (2010) Libraries unlimited. California.
2. Grootenberg (A). Research methodology in Library and information science, (2013) Uxbridge: Koros.
3. Goode (WJ) and Hatt (PK): Methods in social research. McGraw-Hill, (1982) New York.
4. Kothari (C R). Research methodology: Methods & Techniques (Rev. Ed.), (2006) New Age International. New Delhi.
5. Roig (M). Avoiding plagiarism, self-plagiarism, and other questionable writing practices: A guide to ethical writing, (2006).

PRACTICAL-I	M.Sc. Chemistry	2016-2017
M16PCHP01	<b>ORGANIC CHEMISTRY - I</b>	
Credits: 4		

### **PART-I**

1. Separation and analysis of two component organic mixtures by chemical methods.

### **PART-II**

2. Preparations involving single stage.

- (i) Benzoic acid from ethyl benzoate
- (ii) Acetanilide from aniline
- (iii) Acetylsalicylic acid from salicylic acid
- (iv) 2,4,6-Tribromoaniline from aniline
- (v) p-Bromoacetanilide from acetanilide
- (vi) m-Dinitro benzene from nitrobenzene
- (vii) Picric acid from phenol
- (viii) 2-Naphthylbenzoate from 2-naphthol.

### **TEXT BOOKS**

1. N.S. Gnanapragasam and G. Ramamurthy, Organic Chemistry – Lab manual, S.Viswanathan Co. Pvt. Ltd, 1998.
2. J.N. Gurtu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987

### **REFERENCE**

1. Vogel's Text book of Practical Organic Chemistry, 4th Ed, ELBS/Longman, England, 1984.

### **Distribution of marks for practical –I**

Qualitative organic analysis	: 30 marks
Preparation	: 15 marks
Viva-voce in practical	: 10 marks
Record	: 5 marks
Total	: 60 marks
Duration	: 6 hour



PRACTICAL-II	M.Sc. Chemistry	2016-2017
M16PCHP02	<b>INORGANIC CHEMISTRY - I</b>	
Credits: 4		

### PART –I

Semimicro qualitative analysis of mixtures containing two common and two rare cations. The following are the rare to be included: W, Tl, Mo, Te, Se, Ce, Th, Be, Zr, V, U and Li.

### PART – II

- a) Colorimetric analysis: Visual and photometric; determination of iron, nickel, manganese and copper.
- b) Preparation of the following :
  - i)Potassium trioxalatoaluminate (III) trihydrate
  - ii)Tristhiourecopper (I) chloride
  - iii)Potassium trioxalatochromate (III) trihydrate
  - iv)Sodium bis (thiosulphato) cuprate (I)
  - v)Tetramminecopper (II) sulphate
  - vi)Potassium Tetrachlorocuprate (II)

### Reference Books

1. G. Svehla, Vogel's qualitative Inorganic analysis, VI Edition, Orient Longman, 1987.
2. V.V. Ramanujam, Inorganic Semimicro Qualitative analysis. National Publishing Co., 1971.

### Distribution of Marks for Practical –I

Qualitative analysis	:	20 marks
Colorimetric analysis	:	15 marks
Preparation	:	10 marks
Viva – voce in practical	:	10 marks
Record	:	5 marks
Total	:	60 marks
Duration	:	6 hours

PRACTICAL-III	M.Sc. Chemistry	2016-2017
M16PCHP03	<b>PHYSICAL CHEMISTRY - I</b>	
Credits: 4		

Experiments in chemical kinetics, phase rule, Chemical equilibrium and Conductivity measurements:

### DETAILED LIST OF EXPERIMENTS

Typical list of possible experiments are given. Experiments of similar nature and other experiments may also be given. The list given is only a guideline. A minimum of 15 experiments have to be performed in a year.

1. Study the kinetics of acid hydrolysis of an ester, determination of the temperature coefficient of the reaction and determination of the activation energy of the hydrolysis of ethylacetate.
2. Study the kinetics of the reaction between acetone and iodine in acidic medium by half life method and determine the order with respect to iodine and acetone.
3. Study of the saponification of ethylacetate by sodium hydroxide conductometrically and determine the order of the reaction.
4. Determination of association factor of benzoic acid in benzene by distribution method.
5. Study the phase diagram for m-toluidine and glycerine system.
6. Construction of phase diagram for a simple binary system (naphthalene – phenanthrene and benzophenone – diphenylamine)
7. Construction of the phase diagram of the three component of partially immiscible liquid systems (DMSO – Water – Benzene; Water-Benzene –Acetic acid; Ethyl alcohol – Benzene – Water; Acetone-Chloroform – Water; Chloroform – Acetic acid-Water).
8. Determination of equivalent conductance of a weak acid at different concentrations and verify Ostwald's dilution law and calculation of the dissociation constant of the acid.
9. Determination of equivalent conductivity of a strong electrolyte at different concentrations and examine the validity of the Onsager's theory as limiting law at high dilutions.

10. Conductometric titrations of a mixture of HCl and CH<sub>3</sub>COOH against Sodium hydroxide.
11. Compare the relative strength of acetic acid and monochloroacetic acid by conductivity method.

### REFERENCE BOOKS

1. B.P. Levitt (Ed.). Findlay's Practical Physical Chemistry, 9th Edn., Longman, London, 1985.
2. J.N. Gurtu and R.Kapoor, Advanced Experimental Chemistry, Vol I. S. Chand & Co. Ltd., New Delhi, 1980.

### Distribution of Marks for Practical –I

Experiment	:	45 marks
Viva-voce in practica	:	10 marks
Record	:	5 marks
Total	:	60 marks
Duration	:	6 hours

VALULE ADDED	<b>M.Sc. Chemistry</b>	<b>2016-2017</b>
M16PCHVA01	<b>GENERALTRENDS IN APPLIED CHEMISTRY</b>	
Credits: 2		

**Objectives:**

To make the student to understand publications in journals and present a research topic, under the guidance of a professor, in the subject related to Applied Chemistry and his/her broad field of project work in the class room.

**Testing:**

Each student, during, semester-I or II, will give a one hour seminar on a Title of recent trends in applied chemistry taken from current publications in reputed journals. The student will be tested both in subject matter and mode of presentation of the seminar as follows:

**Subject matter - 50 Marks**

- Standard of subject and plan
- Preparation and mastery
- Originality and logical development
- Answers to questions
- Summary and references

**Mode of presentation - 50 Marks**

- Economy of time
- Voice as a tool of communication
- Blackboard use and teaching aids
- Language and diction
- Relating to the audience

MAJOR	M.Sc. Chemistry	2016-2017
M16PCH06	ORGANIC CHEMISTRY-III	
Credits: 5		

### UNIT-I: HETEROCYCLIC CHEMISTRY AND ADDITION TO CARBON-HETERO ATOM MULTIPLE BONDS

Synthesis and reactions of indole, imidazole, thiazole, pyridines, pyrimidine, pyridazine, pyrazine, chromans, chromons, coumarins, carbazoles, uracil, uric acid and xanthines.

Addition to carbon-hetero atom multiple bonds: Mechanisms of metal hydride reduction of carbonyl compounds, acids, esters and nitriles; addition of Grignard reagents and organolithium reagents to carbonyl compounds; mechanisms of formation of hydrates, acetals, oximes and hydrazones on carbonyl compounds, Wittig reaction.

### UNIT-II: FORMATION OF CARBON-CARBON SINGLE BONDS AND C-C $\pi$ BONDS

Formation of carbon- carbon single bonds using organometallic reagents: organolithium, organomagnesium, organocopper, organozinc, organoboron, organosilicon and palladium catalysed coupling reactions. Formation of carbon-carbon  $\pi$  bonds: Wittig olefination- Horner-Wadsworth-Emmons reactions-Peterson olefination- Julia olefination- The Shapiro reaction- Gilbert's reagent.

### UNIT-III: MODERN SYNTHETIC REACTIONS

**Oxidation Reactions:** Chromium and manganese reagents ( $\text{CrO}_3$ ,  $\text{K}_2\text{Cr}_2\text{O}_7$ , PCC, PDC, Sarret reagent, Jones reagent,  $\text{MnO}_2$ ,  $\text{KMnO}_4$ ), Oxygen (singlet and triplet), ozone, peroxides and peracids, lead tetraacetate, periodic acid.  $\text{OsO}_4$ ,  $\text{SeO}_2$ , NBS, chloramine-T, Sommelet oxidation, Oppenauer oxidation, Fenton's reagent, Sharpless epoxidation.

**Reductions:** Catalytic hydrogenation (homogeneous and heterogeneous) catalysts (Pt, Pd, Rh-C, Ni, Ru), Wilkinson catalyst,  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , DIBAL-H, Sodium cyanoborohydride, dissolving metal reactions (Birch reduction). Leukart reaction (reductive amination) Diborane as reducing agent, Meerwein-Ponndorf-Verley reduction, Wolff-Kishner reduction, Clemensen reduction, tributyl tinhydride, stannous chloride, Bakers yeast. Suzuki coupling, Heck reaction, Negishi reaction.

### UNIT-IV: REARRANGEMENTS

Types of rearrangements: Nucleophilic; free radical and electrophilic reactions. Mechanisms: Nature of migration; migratory ability and memory effects, ring enlargement and ring contraction rearrangements Reactions: Wagner-Meerwin and related reactions, Benzil-benzilic acid, Favorskii, Hoffmann and related rearrangements, Beckmann, Neber, Baeyer-Villiger, Stevens, Claisen rearrangements, boron-carbon migration, Non-1,2-rearrangements, Fischer-indole synthesis, Arndt-Eistert synthesis-expansion and contraction of rings.

## UNIT-V: ORGANIC SYNTHESIS BY DISCONNECTION APPROACH

Introduction – Basic Principles of Synthesis of Aromatic Compounds – Disconnection Approach – Functional Group Inter conversions – Synthons – Aromatic Electrophilic and Nucleophilic Substitutions – Strategy I (The order of Events – Some Guidelines) – One-Group CX Disconnections – Strategy II (Chemoselectivity, some Guidelines) – Two-Group Disconnections– Strategy III (Polarity Reversal, Cyclization) – Amine Synthesis (Salbutamol, Fenfluramine) –Protecting the Functional Groups – synthesis of a sweetening agent (Asp-Phe-OMe) – General Strategy of Choosing a Disconnection – Stereoselectivity – Regioselectivity – Alkene synthesis –Use of Acetylenes - Group C-C Disconnections (Alcohols, Carboxylic acids, Carbonyl compounds)

### REFERENCE BOOKS

1. T. L. Gilchrist, Heterocyclic Chemistry, Longman Press, 1989.
2. J. A. Joule and K. Mills, Heterocyclic Chemistry, 4th ed., John-Wiley, 2010
3. Carruthers, Modern Methods in Organic Synthesis, Academic Press, Vol. 1 and 2 (2002)
4. Stuart Warren, Organic Synthesis: The Disconnection Approach, Wiley-India, New Delhi (2007)
5. J. March and M Smith, Advanced Organic Chemistry, 5th ed., John-Wiley and sons, 2001.
6. F. A. Carey and R. Sundberg, Advanced Organic Chemistry, Vol. 1 and 2 (2002)

MAJOR	M.Sc. Chemistry	2016-2017
M16PCH07	<b>INORGANIC CHEMISTRY-III</b>	
Credits: 5		

## UNIT-I

Definition of organometallic compound - 18 electron rule - effective atomic number rule - classification of organometallic compounds - the metal carbon bond types - ionic bond – sigma covalent bond - electron deficient bond - delocalised bond - dative bond - metal carbonyl complexes - synthesis - structure and reactions of metal carbonyls - the nature of M- CO bonding- binding mode of CO and IR spectra of metal carbonyls - metal carbonyls- metal carbonyl anions - metal carbonyl hydrides - metal carbonyl halides - metal carbonyl clusters - Wades rule and isolobal relationship - metal nitrosyls - dinitrogen complexes - dioxygen complexes.

## UNIT - II

Metal alkyl complexes - stability and structure - synthesis by alkylation of metal halides - by oxidative addition - by nucleophilic attack on coordinated ligands - metal alkyl and 18 electron rule - reactivity of metal alkyls - M-C bond cleavage reactions - insertion of CO to M-C bonds - double carbonylation - insertions of alkenes and alkynes - insertions of metals with C-H bonds - alkylidene and alkylidyne complexes - synthesis of alkylidene complexes in low oxidation states and in high oxidation states - bonding in alkylidene complexes - synthesis and bonding in alkylidyne complexes - reactivity of alkylidene and alkylidyne complexes.

## UNIT - III

Alkene complexes - synthesis of alkene complexes by ligand substitution - by reduction and by metal atom synthesis - bonding of alkenes to transition metals - bonding in diene complexes - reactivity of alkene complexes - ligand substitution - reactions with nucleophiles - olefin hydrogenation - hydrosilation - Wacker process - C-H activation of alkenes - alkyne complexes - bonding in alkyne complexes - reactivity of alkynes - alkyne complexes in synthesis - cobalt catalysed alkyne cycloaddition.

## UNIT - IV

Cyclopentadienyl complexes - metallocenes - synthesis of metallocenes - bonding in metallocenes - reactions of metallocenes - Cp<sub>2</sub>Fe/Cp<sub>2</sub>Fe<sup>+</sup> couples in biosensors - bent sandwich complexes - bonding in bent sandwich complexes - metallocene halides and hydrides - metallocene and stereospecific polymerisation of 1-alkenes - cyclopentadiene as a non-spectator ligand - monocyclopentadienyl (half-sandwich) complexes - synthesis and structures of allyl complexes - arene complexes - synthesis - structure and reactivity of arene complexes - multidecker complexes.

## UNIT - V

Organometallic compounds in homogeneous catalytic reactions - coordinative unsaturation - acid-base behaviour reaction - migration of atoms or groups from metal to ligand - insertion reaction - reactions of coordinated ligands - catalytic reactions of alkenes - isomerisation of alkenes - hydrogenation - hydroformylation and hydrosilation of alkenes - alkene polymerisation and oligomerisation - fluxional molecules - The Nobel Prize in Chemistry 2001- Assymmetric synthesis, 2005- Olefins metathesis in organic synthesis and 2010 – Palladium catalysed cross coupling reactions in organic synthesis.

## REFERENCE BOOKS

1. Organometallics 1, complexes with transition metal-carbon -bonds, Bockmann, Oxford science publications, Oxford, 1996.
2. Organometallics 2, complexes with transition metal-carbon -bonds, Bockmann, Oxford science publications, Oxford, 1996.
3. Basic organometallic chemistry, J. Haiduc and J. J. Zuckerman, Walter de Gruyter, Berlin, 1985.
4. Inorganic Chemistry - Principles of structure and reactivity, J. E. Huheey Harper International Edition, Harper and Rone New York, 1978.
5. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, Fourth Edition.



MAJOR	M.Sc. Chemistry	2016-2017
M16PCH08	<b>PHYSICAL CHEMISTRY-II</b>	
Credits: 5		

### **UNIT – I: STATISTICAL THERMODYNAMICS**

Objectives of Statistical thermodynamics – concept of thermodynamical and mathematical probabilities – Distribution of distinguishable and non – distinguishable particles.

Maxwell –Boltzmann, Bose-Einstein and Fermi-Dirac statistics - comparisons

Partition Functions – evaluation of Translational, Vibrational, Rotational and Electronic partition Function – Thermodynamic Functions in terms of partition Function – Application of partition Function to monoatomic and diatomic gases – Statistical expression for equilibrium constant – Calculation of Equilibrium Constant from Partition Function – (isotopic exchange equilibria and dissociation of diatomic molecules) – Heat capacities of Monoatomic crystals – Einstein and Debye theory of heat capacities.

### **UNIT – II: IRREVERSIBLE THERMODYNAMICS**

Postulates of Local equilibrium – Entropy production – Entropy Production in Heat flow – Entropy production in matter flow – Prigogine’s principle of minimum entropy production – Forces and Fluxes – Linear force – flux relation – phenomenological equation – microscopic reversibility and Onsager’s reciprocity relations.

Electrokinetic phenomena – diffusion – Non – equilibrium stationary states.

### **UNIT – III: CHEMICAL KINETICS – III**

Kinetics of complex reactions – reversible reactions, consecutive reactions – Parallel reactions and Chain reactions – General treatment of chain reaction – Chain length – Rice Herzfeld mechanism – explosion limits.

Study of Fast reactions: Luminescence and energy transfer process – Study of kinetics by relaxation methods-temperature and pressure jump methods - Stopped flow technique, flash photolysis and Crossed molecular beam method.

### **UNIT – IV: QUANTUM CHEMISTRY – III**

Theory of chemical bonding – Born – Oppenheimer approximation – LCAO – MO approximation for hydrogen molecule ion and Hydrogen – Valence Bond theory of Hydrogen molecule – Concept of Hybridisation – sp, sp<sup>2</sup> and sp<sup>3</sup> hybridisation – Huckel Molecular orbital (HMO) theory for conjugated  $\pi$ - system – applications to simple systems – (Ethylene, butadiene and benzene) – Physical Significance of HMO coefficients – Self consistent field approximation – Hartree’s and Hartree – Fock Self Consistent field theory – Slater type orbitals – Slater rules.

## UNIT – V: SPECTROSCOPY – II

NMR spectroscopy – theory – nuclear zeeman effect- chemical shift – Spin-spin coupling – NMR of simple AX and AMX type molecules – Calculation of coupling constants -<sup>13</sup>C-NMR – a brief discussion of Fourier Transformation.

ESR Spectroscopy – Theory – hyperfine interactions – Spin densities – McConnell relationship – selection rules in ESR – ‘g’ value and coupling constants.

### TEXT BOOKS:

1. Gurudeep raj, Advanced Physical Chemistry, Goel Publishing House, Meerut.
2. M.C. Gupta, Statistical Thermodynamics, Wiley Eastern, New Delhi, 1990.
3. R. Hasse, Thermodynamics of Irreversible Process, Addison Wesley, Reading, Mass 1969.
4. I. Prigogine, Introduction to Thermodynamics of Irreversible Process, InterScience, New York, 1961.
5. J. Rajaram and J.C. Kuriakose, Kinetics and Mechanism of Chemical Transformations, Macmillan India Ltd., 1993.
6. K.J. Laidlar, Chemical Kinetics, Harper and row, New york. 1987.
7. R.K. Prasad, Quantum Chemistry, Wiley Eastern, New Delhi, 1992.
8. M.W. Hanna, Quantum Mechanics in Chemistry, W.A. Benjamin Inc, London 1965.
9. C.N. Banwell, Fundamentals of Molecular Spectroscopy, Mc Graw Hill, Newyork, 1966.
10. A. Carrington and A.D. McLachlan, Introduction to Magnetic Resonance, Harper and Row, New york (1967)

### REFERENCE BOOKS

1. M. Dole, Statistical Thermodynamics, Prentice Hall, New York, 1954.
2. B.J. McClelland, Statistical Thermodynamics, Chapman and Hall, London 1973.
3. N.O. Smith, Elementary, Statistical Thermodynamics, a Problem approach, Pleunum Press, New York, 1980.
4. R.G. Frost and Pearson, Kinetics and Mechanism, Wiley New York, 1961.
5. J.W. Moore, and R.G. Pearson, Kinetics and Mechanism, 1981.
6. C. Capellos and B.H.J. Bielski, Kinetics Systems, Wiley inter science, New York, 1972.
7. I. Amdur and C.G. Hammes, Chemical Kinetics, Principle and Selected Topics, McGraw Hill, New York, 1968.
8. G.M. Harris, Chemical Kinetics, D.C. Heath and Co, 1966.
9. A.K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill.
10. D.A. McQuarrie, Quantum Chemistry, University Science Books, Mill Valley, California (1983).

11. P.W. Atkins, Molecular Quantum Mechanics, Oxford University Press, Oxford, 1983.
12. J.N. Murrell, S.F.A. Kettle and J.M. Tedder, The Chemical Bond, Wiley.
13. Raymond chang, Basic Principle of Spectroscopy, McGraw Hill Ltd., New York (1971).
14. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1962.
15. W. Kemp, NMR in Chemistry, Mac Millan Ltd., (1986).
16. K.P. McLauchlan, Magnetic Resonance, Oxford Chemistry series, Oxford, (1972).
17. F.A. Rushworth and D.P. Tunstall, Nuclear Magnetic Resonance, Gordon and Breach Science Publishing, New York, (1973).
18. J.K.M. Sanders and B.K. Hunther, Modern NMR Spectroscopy, A guide for chemists, Oxford University press, Oxford, (1987).

ELECTIVE-III	M.Sc. Chemistry	2016-2017
M16PCHE09	<b>ELECTROCHEMISTRY, SPECTROSCOPY AND ANALYTICAL TECHNIQUES</b>	
Credits: 4		

### **UNIT – I: ELECTROCHEMISTRY – I**

Ions in solutions – Debye – Huckel theory of strong electrolytes – Debye – Huckel – Onsager equation – verification and limitation – Debye – Huckel limiting law and its extension. Electrode – Electrolyte interface - adsorption at electrified interface – electrical double layers – Electro capillary phenomena – Lippmann capillary equation – structure of double layers – Helmholtz Perrin, Gouy-Chapman and Stern models of electrical double layers – electro kinetic Phenomena – Tiselius method of separation of proteins – Membrane potential.

### **UNIT – II: ELECTROCHEMISTRY – II**

Mechanism of electrode reactions – Polarisation and Over Potential – the Butler Volmer equation for one step and multi step electron transfer reactions – significance of equilibrium exchange current density and symmetry factor – transfer coefficient and its significance – Theory and applications of dropping mercury electrode – Polarography, Amperometry and Cyclic voltametry – Principles and applications – mechanism of Hydrogen and Oxygen evolution reactions.

### **UNIT – III: ELECTROCHEMISTRY – III**

Electrochemical inorganic and organic reactions of technological interest (at least one example in each) – Corrosion and Passivation of metals – construction of Pourbaix and Evans diagrams – Prevention of Corrosion.

Electrochemical energy systems – Primary and Secondary batteries – (dry cells, lead acid - storage batteries, silver zinc cell, nickel cadmium battery, mercury cell) – Fuel cells – Electrodeposition – Principles and applications.

### **UNIT – IV: EPR SPECTROSCOPY AND MOSSBAUER SPECTROSCOPY**

Theory : EPR spectra of VO (II), Mn (II), Co (II), Ni (II) and Cu (II) complexes; covalency of metal – ligand bonding by EPR; John-teller distortions in Cu(II) complexes.

Mossbauer Spectroscopy – Doppler effect; isomer effect; electron – neutron hyperfine interactions; Quadrupole interactions and magnetic interactions; simple applications to Iron and Tin compounds.

### **UNIT-V: ANALYTICAL TECHNIQUES**

Chromatography – Gas liquid chromatography – Principle, retention volumes; instrumentation; carrier gas; columns preparations; stationary phase; detectors – thermal conductivity, flame ionization, electron capture; applications of GLC.

High Performance liquid chromatography – scope; column efficiency; instrumentation; pumping systems; columns; column packing; detectors; applications.

## REFERENCE BOOKS

1. S. Glasstone, Introduction to Electro Chemistry, Affiliated East West Press, NewDelhi, 1960.
2. D.R. Craw, Principles and applications of Electro chemistry, Chapman andHall, 1991.
3. J. Robbins, Ions in solution – An Introduction to Electro chemistry, ClarendonPress, Oxford (1972).
4. D.A. Skoog and D.M. West, Fundamentals of Analytical Chemistry, Holt Rinehart and Winston Publications, IV Edn, 1982.
5. D.A. Skoog, Principles of Instrumental Analysis, Saunders College Pub. Co, III Edn., 1985.
6. R.S. Drago, Physical Methods in Chemistry, Reinhold, New York, 1968.

ELECTIVE-III	M.Sc. Chemistry	2016-2017
M16PCHE10	ADVANCED INDUSTRIAL INORGANIC COMPOUNDS	
Credits: 4		

### Unit- I

Ceramics – classification, optical waveguides (optical fiber), sol-gel formation for low temperature ceramic formation. Non-oxide ceramics – general aspects, silicon carbide, silicon nitride and boron nitride ceramics. Fabrication of ceramic materials and its challenges.

### Unit -II

Carbon fibers: introduction, manufacture, applications and economic importance. SiC-coated carbon fibers. Aluminium oxide coated fibers; their manufacture and applications. Zeolites: Natural and synthetic zeolites, manufacture of synthetic zeolites from different sources, pelletization, dehydration and applications.

### Unit -III

Inorganic pigments: white pigments: TiO<sub>2</sub> pigment, its manufacture, post-treatment and applications; ZnO white, lithopone and ZnS pigments. Coloured pigments: iron oxide pigments – manufacture, oxidation processes and applications.

### Unit -IV

Silicon: metallurgical grade, ferrosilicon and electronic grade silicon, manufacture and applications. Silicones & poly(organo siloxanes) (POS): manufacture, linear and branched POS, high molecular weight POS; silicone oil, emulsion, rubbers and resins.

### Unit V

General characteristics, degree of polymerization, catenation and heterocatenation, SN chain one dimensional conductor, isopoly and heteropoly acids (polyoxometallates) and their characteristics and applications (introductory level), phosphazene polymers; Metal clusters: dinuclear, trinuclear, tetranuclear and hexanuclear clusters and their synthesis and properties.

### REFERENCE BOOKS

1. H.R. Allcock, Introduction to Materials Chemistry, Wiley, 2008.
2. S.K. Agarwala, Keemti Lal, Advanced Inorganic Chemistry, Pragati Prakashan, 10th edn., 2011.
3. A.R. West, Solid State Chemistry and its applications, Wiley, 2004.
4. M.G. Arora, M. Singh, Industrial Chemistry, Anmol Publications, Reprint 2004.
5. Harish Kumar, Industrial Chemistry, Sarup & Sons Reprint 2002.
6. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry, Pearson Education Asia, Reprint 2001.

7. F.A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, John Wiley & Sons, 5th Edn., 1988.
8. B.E. Douglas, D.H. McDaniel and J.J. Alexander, *Concepts and Models of Inorganic Chemistry*, John Wiley & Sons, 2 Edn. 1983.
9. I. V. Kozhevnikov, *Catalysis by Heteropoly Acids and Multicomponent Polyoxometalates in Liquid-Phase Reactions*, *Chem. Rev.* 1998, 98, 171-198.
10. D. E. Katsoulis, *A Survey of Applications of Polyoxometalates*, *Chem. Rev.* 1998, 98, 359-387.

ELECTIVE-III	M.Sc. Chemistry	2016-2017
M16PCHE11	<b>NUCLEAR CHEMISTRY</b>	
Credits: 4		

### Unit I

Discovery – types of decay – decay kinetics – half-life period, mean life, parentdaughter decay – growth relationship – secular and transient equilibrium; Units of radioactivity; alpha, beta and gamma decay; Theory of decay, energies and properties – artificial radioactivity. Detectors: ionization chamber, electron pulse counter, scintillation detectors.

### Unit II

Bathe's notation – types of nuclear reactions: The compound nucleus theory – reaction cross section, transmutation reactions, elastic and inelastic scattering, spallation, fragmentation, stripping and pick-up; fission, fusion, photonuclear reactions and thermonuclear reactions.

### Unit III

The fission energy – reproduction factor; Classification of reactors based on moderators, coolants, phase of fuel and generation. Principle of thermal nuclear reactors: The four factor formula, reactor power, critical size of a thermal reactor, excess reactivity and control. Breeder reactor India's nuclear energy programmes – reprocessing of spent fuels.

### Unit IV

Radiation chemistry – passage of radiation through matter – units for measuring radiation absorption – radiation dosimetry – radiolysis of water – free radicals in water radiolysis – chemical dosimetry: Radiolysis of Fricke Dosimeter solution – Radiation induced colour centres in crystals – Effects of radiation with matter. Radiolysis of inorganic gases, organic gases, organic compounds, solids and polymers – Annealing of radiation damage.

### Unit V

Application of radioisotopes: probing by isotopes, reactions involved in the preparation of radioisotopes. The Szilard-Chalmers' reaction – Radiochemical principles in the use of Tracers – Applications of radioisotopes as tracers – chemical investigations, analytical applications, agricultural and industrial applications – Neutron activation analysis – Carbon and rock dating .

## REFERENCE BOOKS

1. S. Glasstone, Source book on atomic energy, East West press, 3<sup>rd</sup> Edn. 1967.
2. H.J. Arniker, Essentials of Nuclear Chemistry, New Age International, Reprint 2009.
3. M.G. Friedlander, J.M. Kennedy, E.S. Macian and J.M. Miller, Nuclear and Radiochemistry, 3<sup>rd</sup> Edn. John Wiley & Sons, 1981.
4. M.G. Arora and M. Singh, Nuclear Chemistry, Anmol Publications, 1994.
5. E.S.Gilreath, Fundamental concepts of Inorganic Chemistry, McGraw Hill 17<sup>th</sup> print 1982.



ELECTIVE-III	M.Sc. Chemistry	2016-2017
M16PCHE12	<b>CATALYSIS</b>	
Credits: 4		

### Unit-I

Catalysis phenomenon – mode of action of catalysts – classification of catalysts – Comparison of Homogeneous and Heterogeneous Catalysis. Homogeneous catalysis – general mechanisms; acid-base catalysis – catalytic activity, mechanisms and salt effects. Enzyme catalysis – influence of substrate concentration, pH, temperature, and enzyme mechanisms. Kinetics of inhibition – chain reaction, enzyme catalyzed reactions.

### Unit-II

Catalysis in molecular-scale cavities – structure of crystalline solids – zeolites – families of zeolites; adsorption and diffusion in zeolites – catalysis by zeolites containing metal complexes and clusters; non-zeolite molecular sieves – clays and other layered materials. Catalysis – catalysts for PTC – mechanism and benefits of PTC – PTC reactions – selected industrial processes with PTC.

### Unit-III

Micellar catalysis: effects of micelles on chemical reactions, characteristics of enzymatic reactions, micelle-catalyzed reactions, inhibition in micellar solutions; reverse micelles and microemulsions – catalysis in thermal and photochemical reactions.

### Unit-IV

Electrocatalysis – introduction to electrocatalysis and fuel cells – industrial application of catalysis – petroleum refining – distillation, cracking, reforming, hydrotreating, Alkylation and isomerization, ethylene-based processes – ethylene oxide and ethylene glycol, polyethylene, vinyl chloride and PVC; Propylene-based processes – acrylic acid and acrylonitrile, Ziegler-Natta chemistry; C<sub>5</sub>-based processes – butadiene, isobutylene.

### Unit-V

Surface catalysis – introduction – mechanism of surface reactions: Langmuir Hinshel wood & -Rideal mechanisms; surface structures – single crystal surface of metals, high-surface area amorphous solids; adsorption; functionalized surfaces; catalysis on functionalized surfaces: connection to molecular catalysis; catalysis on metal surfaces, metal oxide surfaces, mixed metal oxides, metal sulfides.

## REFERENCE BOOKS

1. B. C. Gates, Catalytic Chemistry, John Wiley & Sons, Inc., 1992.
2. J. C. Kuriacose, Catalysis, Macmillan India Ltd., New Delhi, 1991.
3. M. Gratzel, K. Kalyanasundaram, Eds., Kinetics and Catalysis in Microheterogeneous Systems, Marcel Dekker, New York, 1991.
4. K. Kalyanasundaram, Photochemistry in Microheterogeneous Systems, Academic Press, Orlando, 1987.
5. K. J. Laidler, Chemical Kinetics, 3rd Edition, Pearson Education Pte., Ltd., 2005.
6. P. H. Emmett, Catalysis, Vol. I and II, Reinhold Corp., New York, 1954.
7. J. M. Smith, Chemical Engineering Kinetics, McGraw Hill, 1971.
8. J. Hagen, Industrial Catalysis: A Practical Approach, 2nd Edition, Wiley-VCH, 2006.

MAJOR	M.Sc. Chemistry	2016-2017
M16PCH09	<b>ORGANIC CHEMISTRY-IV</b>	
Credits: 5		

### UNIT-I: PERICYCLIC REACTIONS

Molecular orbital symmetry; frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system; classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams; FMO and transition state aromaticity approach; selection rules.

Cyclo addition reactions-(4+2), (2+2) cyclo addition -selectivity-substituent effect-inverse electron demand Diels-Alder reactions-1,3-dipolar cycloadditions of ozone, diazomethane and nitrile oxide and chelotropic reactions.

### UNIT-II: ELECTROCYCLIC REACTIONS AND SIGMATROPIC REARRANGEMENTS

Electro cyclic reactions: conrotatory and disrotatory motions; ring opening and ring closing reactions-  $4n$ ,  $4n+2$  and allyl systems.

Sigmatropic rearrangements: (1,3), (1,5), (1,7), (3,3) and (5,5)-carbon migrations, degenerate sigmatropic rearrangements.

### UNIT-III

Problems on the applications of cycloaddition, electrocyclic and sigmatropic reaction to be discussed and assigned home works.

### UNIT-IV: LAWS OF PHOTOCHEMISTRY AND PHOTOPRIMARY PROCESSES

Interaction of Electromagnetic radiation with Matter-Types of excitations – Laws of Photochemistry – Grothus and Draper law – Lambert and Beer's law – Einstein law – Quantum yield – Photo primary processes, fate of the Excited molecule – State energy diagrams – Fluorescence – Fluorescence life times – phosphorescence life times – Quenching – Stern – Volmer equation – Inter molecular processes – Photosensitisation – Predissociation – Fluorescence and structure – Triplet state and phosphorescence emission.

### UNIT-V: PHOTOCHEMICAL REACTIONS

Light absorption – Experimental techniques – Electronic transitions – Frank – Condon principle – Jablonski diagrams – Intersystem crossing – Energy transfer – Molecular orbital view of excitation – The Geometry of excited states – Reactivity of Electronically excited ketones –  $\alpha$  - cleavage -  $\gamma$  - hydrogen transfer Norrish Type I, Type II, Type III reactions – Photoreduction – Oxetate formation – Reactivity of  $\pi$ ,  $\pi^*$  excited ketones – Photochemistry of  $\alpha$ ,  $\beta$  - unsaturated ketones – Optical pumping – Dienone phenol rearrangement.

**REFERENCE BOOKS:**

1. Fundamentals of Photochemistry – K.K.Rohatgi – Mukherjee (Revised Edition) New age International publications, Reprint 2002.
2. Physical Chemistry – Robert A.Alberty (Sixth edition) – Wiley Eastern Limited Reprint 1987.
3. F. A. Carey and R. Sundberg, Advanced Organic Chemistry, Vol. 1 & Vol.2 and 2 (2002).
4. J. March and M Smith, Advanced Organic Chemistry, 5thed., John-Wiley and sons, 2001.
5. Principles of Organic synthesis, R.O.C. Norman, J.M. Coxon, 3rd Edition., Chapman & Hall, (1993).

MAJOR	M.Sc. Chemistry	2016-2017
M16PCH10	<b>INORGANIC CHEMISTRY-III</b>	
Credits: 5		

## UNIT - I

The growth and form of crystals - the crystal systems and Bravais lattices - Miller indices and labelling of planes - symmetry properties - crystallographic point groups and space groups - fundamentals of X-ray diffraction - powder and rotating crystal methods - systematic absences and determination of lattice types - analysis of X-ray data for cubic system - structure factor and Fourier synthesis - electron and neutron diffraction and structure determination.

## UNIT - II

Types of solids - close packing of atoms and ions - bcc, fcc and hcp voids - Goldschmidt radius ratio - derivation - its influence on structures - structures of rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluoroite - antiferite - diamond and graphite - spinel - normal and inverse spinels and perovskite - lattice energy of ionic crystals - Madelung constant - Born-Haber cycle and its applications.

## UNIT - III

Metallic state - free electron and band theories - non - stoichiometry - point defects in solids - Schottky and Frenkel defects - linear defects - dislocations - effects due to dislocations - electrical properties of solids - insulators - intrinsic semiconductors - impurity semiconductors (n and P type) and superconductors - elementary study of liquid crystals.

## UNIT - IV

Nucleus: nuclear structure - stability of nuclei - packing fraction - even - odd nature of nucleons - n/p ratio - nuclear potential - binding energy and exchange forces - shell model and liquid drop model. Decay of radionuclei: rate of decay - determination of half-life period - secular equilibrium and decay series. Modes of decay: alpha, beta, gamma and orbital electron capture - nuclear isomerism - internal conversions - Q value - nuclear cross section - threshold energy and excitation functions. Particle acceleration and counting techniques: linear accelerator - cyclotron and synchrotron - betatron - G. M. counter - proportional and scintillation counters.

## UNIT - V

Different type of nuclear reactions with natural and accelerated particles - transmutation - stripping and pick-up - spallation - fragmentation, etc. - fission - characteristics of fission reaction - product distribution and theories of fission - fissile and fertile isotopes - U235, U238, Th232 and Pu239 - atom bomb - nuclear fusion - stellar energy - synthesis of new elements - principles underlying the usage of radioisotopes in analysis - agriculture - industry and medicine - mechanism of chemical reactions - uses of radioisotopes in analytical chemistry - isotopic dilution analysis - neutron activation analysis and dating methods.

## REFERENCES

1. W.J.Moore – Physical Chemistry
2. L.V.Azroff – Introduction to solids
3. W.E.Addision – structural principles of Inorganic Chemistry
4. N.B.Hannay – Solid state chemistry
5. R.A.Alberty – Physical chemistry
6. S.Glasstone – Source book on atomic energy
7. G.Friedlander, J.W.Kennedy, - Nuclear and Radiochemistry
8. H.J.Arnikaar – Essentials of Nuclear chemistry.

PRACTICAL – IV	M.Sc. Chemistry	2016-2017
M16PCHP04	<b>ORGANIC CHEMISTRY – II</b>	
Credits: 3		

## PART-I

### 1. Estimations

- Phenol and aniline
- Ketones (ethyl methyl ketone)
- Sugars (Glucose)
- Ascorbic acid (Vitamin-C tablets)
- Amino groups (aniline)
- Nitro groups (aromatic nitro compounds)
- Amino acids (Glycine)

## PART-II

### A. Two stage preparations

- p-Bromoacetanilide from Aniline
- p-Nitroaniline from Acetanilide
- 1,3,5-Tribromobenzene from Aniline
- Acetyl salicylic acid from Methyl salicylate
- Benzilic acid from Benzoin
- m-Nitroaniline from Nitrobenzene
- $\beta$ -Naphthol from Naphthalene

## TEXT BOOKS

- N.S. Gnanapragasam and G. Ramamurthy, Organic Chemistry – Lab manual, S. Viswanathan Co. Pvt. Ltd, 1998.
- J.N. Gurtu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987

## REFERENCE

- Vogel's Text book of Practical Organic Chemistry, 4thEdn, ELBS/Longman, England, 1984.

PRACTICAL – V	M.Sc. Chemistry	2016-2017
M16PCHP05	<b>INORGANIC CHEMISTRY – II</b>	
Credits: 3		

### **PART-I: Quantitative analysis**

Quantitative analysis of the following mixture

1. Iron and magnesium
2. Iron and nickel
3. Copper and nickel
4. Copper and Zinc

### **PART-II**

Preparations of the following:

1. Sodium hexanitrocobaltate (III)
2. Sodium Trisoxalatoferrate (III)
3. Prussian blue  $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$
4. Bis (acetylacetonato) Copper (II)
5. Hexamminecobalt (III) chloride
6. Hexamminenickel (II) chloride

### **REFERENCE BOOKS:**

1. G. Svehla, Vogel's qualitative Inorganic analysis, VI Edition, Orient Longman, 1987.
2. V.V. Ramanujam, Inorganic Semimicro Qualitative analysis. National Publishing Co., Chennai. 1971.
3. J. Basset, R.C. Denney, G.H. Jeffery and J. Mendham Vogel's Text book of quantitative inorganic analysis, IV Edition, ELBS, 1985.
4. W.G. Palmer, Experimental Inorganic Chemistry, Van Nostrand Reinhold Co., London, 1972.
5. D.N. Grindley, An advanced course in practical Inorganic Chemistry, Butterworths, 1964.



PRACTICAL – VI	M.Sc. Chemistry	2016-2017
M16PCHP06	PHYSICAL CHEMISTRY – II	
Credits: 3		

### Experiments in Electrochemistry, Polarography and Chemical Kinetics.

#### EMF Measurements

1. Determination of standard potentials (Cu and Ag)
2. Determination of thermodynamic quantities from EMF measurements
3. Potentiometric titrations.
4. Determination of pH and calculation of pKa.
5. Determination of stability constant of complex.
6. Determination of solubility product of a sparingly soluble salt, Redox titrations.
7. Precipitation titration of mixture of halides by emf measurements.

#### DETAILED LIST OF EXPERIMENTS

Typical list of possible experiments are given. Experiments of similar nature and other experiments may also be given. The list given is only a guideline. A minimum of 15 experiments have to be performed.

1. Determination of the activity coefficient of an electrolyte at different molalities by emf measurements.
2. Determination of the dissociation constant of acetic acid by titrating it with sodium hydroxide using quinhydrone as an indicator electrode and calomel as a reference electrode.
3. Determination of the strength of a given solution of KCl using differential potentiometric titration technique.
4. Determination of the pH of the given solutions with the help of the indicators using buffer solutions and by colorimetric method.
5. Determination of the pH of a given solution by emf method using hydrogen electrode and quinhydrone electrode.
6. Determination of the composition and instability constant of a complex by mole ratio method.
7. Calculation of the thermodynamic parameters for the reaction  

$$\text{Zn} + \text{H}_2\text{SO}_4 \text{ -----} \rightarrow \text{ZnSO}_4 + \text{H}_2 \text{ by emf method.}$$
8. Determination of the formation constant of silver ammonia complex and stoichiometry of the complex potentiometrically.
9. Solubility and solubility products by emf method.
10. Determination of the activity coefficient of Zinc ions in the solution of 0.002 M Zinc sulphate using Debye - Huckel Limiting law.
11. Determination of solubility product of Silver bromide and calculate its solubility in water and 0.1 M and 0.01 M  $\text{KBrO}_3$  using Debye- Huckel limiting law.

12. Determination of the electrode potentials of Zn and Ag electrodes in 0.1 M and 0.001M solutions at 298 K and find the standard potentials for these electrodes and test the validity of Nernst equations.
13. Study the inversion of cane sugar in presence of acid using polarimeter.
14. Determination of the rate constant and order of reaction between potassium persulphate and potassium iodide and determine the temperature coefficient and energy of activation of the reaction.
15. Study the primary salt effect on the kinetics of ionic reactions and test the Bronsted relationship (iodide ion is oxidized by persulphate ion.)
16. Determination of the viscosities of mixtures of different compositions of liquids and find the composition of a given mixture.
17. Determination of the partial molar volume of glycine/methanol/formic acid/ sulphuric acid by graphical method and by determining the densities of the solutions of different compositions.
18. Study the surface tension – concentration relationship of solutions (Gibb's equation)

## REFERENCE BOOKS

1. B.P. Levitt (Ed.). Findlay's Practical Physical Chemistry, 9th Edn., Longman, London, 1985.
2. J.N. Gurtu and R.Kapoor, Advanced Experimental Chemistry, Vol I. S. Chand & Co. Ltd., New Delhi, 1980.

PROJECT	M.Sc. Chemistry	2016-2017
M16PCHPR1	<b>PROJECT</b>	
Credits: 4		

**Objectives:**

To make the student to understand and present a research finding on a topic in the subject related to Chemistry under the guidance of a Department Staff.

**Testing:**

The student will be tested both in subject matter of the report and the mode of presentation in the viva-voce examination.

The viva-voce examination, on the project work done, will be conducted by two examiners (Project guide & an external examiner appointed by the Controller of examination)

**Project report: 150 Marks**

- Standard of subject and plan
- Preparation and mastery
- Originality and logical development
- Summary and references

**Viva-voce: 50 Marks**

- Economy of time
- Communication
- Blackboard use and teaching aids
- Language and diction
- Answer to questions

EDC	M.Sc. Chemistry	2016-2017
M16PCHE01	<b>GREEN MANUFACTURING TECHNOLOGY</b>	
Credits: 4		

### UNIT-I

Introduction to green chemistry: Green chemistry-relevance and goals, Anastas' twelve principles of green chemistry - Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

### UNIT-II

Microwave activation – advantage of microwave exposure – specific effects of microwave – Neat reactions – solid supports reactions – Functional group transformations – condensations reactions – oxidations – reductions reactions – multi-component reactions.

### UNIT-III

Ionic liquids and PTC Introduction – synthesis of ionic liquids – physical properties – applications in alkylation – hydroformylations – epoxidations – synthesis of ethers – Friedel-Craft reactions – Diels-Alder reactions – Knoevenagel condensations – Wittig reactions – Phase transfer catalyst - Synthesis – applications.

### UNIT-IV

Supported catalysts and bio-catalysts for Green chemistry Introduction – the concept of atom economy – supported metal catalysts – mesoporous silicas – the use of Biocatalysts for green chemistry.

### UNIT-V

Fermentations and biotransformations – fine chemicals by microbial fermentations – vitamins and amino acids – Baker's yeast mediated biotransformations – Bio-catalyst mediated Baeyer-Villiger reactions – Microbial polyester synthesis.

### REFERENCE BOOKS

1. Green Chemistry – Environmentally benign reactions – V. K. Ahluwalia. Ane Books India (Publisher). (2006). Green Chemistry – Designing Chemistry for the Environment – edited by Paul T. Anastas & Tracy C. Williamson. Second Edition, (1998).
2. Green Chemistry – Frontiers in benign chemical synthesis and processes- edited by Paul T. Anastas & Tracy C. Williamson. Oxford University Press, (1998).
3. Green Chemistry – Environment friendly alternatives- edited by Rashmi Sanghi & M. M. Srivastava, Narora Publishing House, (2003).

EDC	M.Sc. Chemistry	2016-2017
M16PCHE02	<b>NANO TECHNOLOGY IN CHEMICAL INDUSTRY</b>	
Credits: 4		

### UNIT – I

Nanoscale, nanomaterials –definition. Types of nanomaterials – quantum wells, quantum wires, quantum dot. Different types of nano structures – nanoclusters, nanocrystals, nanowires and nanotubes, definition of nanotechnology, nanoscience and nanochemistry. Significance of the nanoscale. Factors responsible for the special properties of nanomaterials. Nanotechnology and health issues - risks from nanoparticles and nanosafety. Nanotechnology and environmental issues.

### UNIT – II

A few important methods of synthesis of nanomaterials – Laser Ablation, Sonication, phase – transfer methods and sol – gel method. Application of nanotechnology – medicine diagnostics, drug delivery, food and drinks, cosmetics, textiles, sports / outdoor, filtration chemical industry, catalysis, electronic, displays.

### UNIT III

Sol gel processing-Solvothermal, hydrothermal, precipitation, Spray pyrolysis, Electro spraying and spin coating routes, Self-assembly, self-assembled monolayers (SAMs). Langmuir-Blodgett (LB) films, micro emulsion polymerization- templated synthesis, pulsed electrochemical deposition.

### UNIT IV

Vapor deposition and different types of epitaxial growth techniques (CVD,MOCVD, MBE,ALD)- pulsed laser deposition, Magnetron sputtering - lithography :Photo/UV/EB/FIB techniques, Dip pen nanolithography, Etching process :Dry and Wet etching, micro contact printing.

### UNIT V

Zeolites, mesoporous materials, nanomembranes - Carbon nanotubes and graphene - Core shell and hybrid nanocomposites. Overview of nanomaterials properties and their applications, Molecular Electronics and Nanoelectronics – Nanobots- Biological Applications – Quantum Devices – Nanomechanics - Photonics- Nano structures as single electron transistor –principle and design.

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2. S.P. Gaponenko, *Optical Properties of semiconductor nanocrystals*, Cambridge University Press, 1980.
3. W.Gaddand, D.Brenner, S.Lysherski and G.J.Infrate(Eds.), *Handbook of NanoScience, Engg. and Technology*, CRC Press, 2002.

4. K. Barriham, D.D. Vvedensky, Low dimensional semiconductor structures: fundamental and device applications, Cambridge University Press, 2001.
5. G. Cao, Nanostructures & Nanomaterials: Synthesis, Properties & Applications, Imperial College Press, 2004.
6. J. George, Preparation of Thin Films, Marcel Dekker, Inc., New York. 2005.