

**M.Sc. Chemistry  
Courses offered**

<b>Semester</b>	<b>Subject code</b>	<b>Title of the paper</b>	<b>Hours/week</b>	<b>Credit</b>
<b>I</b>	PG1711	Core I Organic Chemistry –I	6	4
	PG1712	Core II Inorganic Chemistry – I	6	5
	PG1713	Core III Physical Chemistry – I	6	4
	PG1714 PG1715	Elective I – (a) Instrumental Methods of Analysis (b) Electrochemistry	6	4
	PG17P1	Practical I- Organic Chemistry	6	-
<b>II</b>	PG1721	Core IV Organic Chemistry – II	6	4
	PG1722	Core V Inorganic Chemistry – II	6	5
	PG1723	Core VI Physical Chemistry – II	6	4
	PG1724 PG1725	Elective II (a) Research Methodology (b) Nuclear Chemistry	6	4
	PG17P1	Practical I - Organic Chemistry	-	5
	PG17P2	Practical II - Inorganic Chemistry	6	5
	LST172	Life Skill Training (LST) – I	-	1
<b>III</b>	PG1731	Core – VII- Organic Chemistry – III	6	5
	PG1732	Core – VIII - Physical Chemistry – III	6	4
	PG1733 PG1734	Elective III – (a) Advanced Topics in Chemistry (b) Medicinal Chemistry	6	4
	PG17P3	Practical III Gravimetric analysis and Inorganic preparations	4	-
	PG17PR	Project and Viva	8	4
<b>IV</b>	PG1741	Core – IX - Organic Chemistry – IV	6	4
	PG1742	Core – X -Inorganic Chemistry – III	6	5
	PG1743	Core – XI- Physical Chemistry – IV	6	4
	PG1744 PG1745	Elective IV – (a) Energy for the Future (b) Nanochemistry	6	4
	PG17P3	Practical III Gravimetric analysis and Inorganic preparations	-	4
	PG17P4	Practical IV Physical Chemistry	6	5
	LST174	Life Skill Training (LST) – II	-	1
	STP171	Summer Training Programme	-	1
		<b>TOTAL</b>	<b>120</b>	<b>90</b>

**Semester I**  
**Organic Chemistry I**  
**Sub. Code: PG1711**

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

**Objectives:**

1. To gain knowledge on polarization effects and hyper conjugations
2. To understand the stereochemistry of compounds.
3. To know about the conformations of organic compounds.
4. To enable the students gain knowledge about the methods of addition in alkenes.
5. To get information about various reactions and their mechanisms.

**Unit I: Electron Displacement and Reactive Intermediates**

Polarization effects: Inductive effect, Mesomeric effect, types and impact on the physico-chemical characteristics of molecules and dissociation constants of acids and bases, Tautomerism. Comparison of mesomerism and tautomerism, Hyperconjugation, Steric effects in molecules and their impact Preparation and stability of carbocations, carbanions and free radicals. Preparation structure stability and reactions of carbenes and nitrenes. Electron Donor Acceptor complexes - types, nature and applications.

**Unit II: Stereochemistry**

Concept of chirality. Newman, Sawhorse and Fischer projections and their conversion. Enantiotopic, diastereotopic hydrogens and prochiral centres. Axial and planar chirality - ansa compounds and cyclophanes. Stereochemistry of compounds containing two dissimilar asymmetric carbons.

Optical activity of biphenyls, allenes and spiranes. Optical isomerism of nitrogen and sulphur compounds.

Stereospecific and stereoselective synthesis. Asymmetric synthesis. Cram's rule - open chain, cyclic and dipolar model. Prelog's rule.

**Unit III: Conformational Analysis**

Conformation: Definition, Differences between configuration and conformation, Conformation of simple acyclic systems. Effects of conformation on reactivity of acyclic system - electrophilic addition, nucleophilic addition, cis- and trans- addition, E<sub>2</sub> elimination and cis-elimination.

Conformation of cyclic systems up to 6 membered rings, Conformational analysis of mono and di-substituted cyclohexanes. Effects of conformation on reactivity of cyclic systems involving saponification, esterification, S<sub>N</sub><sup>1</sup> and S<sub>N</sub><sup>2</sup> reactions.

Conformation equilibrium. Curtin-Hammet principle. Conformation of decalin, perhydrophenanthrene and perhydroanthracene.

**Unit IV: Addition to multiple bonds**

Mechanism and stereochemical factors in reactions like addition of hydrogen halides, hypohalous acids, hydroboration, hydroxylation and epoxidation.

Mechanism and applications of Michael addition, Diels' Alder reaction, Knoevenagal reaction, Mannich reaction, Stork-enamine reaction, Grignard reaction, Darzen's reaction, Reformatsky reaction and Wittig reaction.

## Unit V: Organic Reaction Mechanism and Methods

Reaction mechanism: Energy diagram of simple organic reactions, transition state and intermediate. Kinetic and Thermodynamic requirements of reactions. Baldwin rules for ring closure, Hammond postulate, microscopic reversibility and control of product formation.

Primary and secondary isotope effect. Testing and Trapping of intermediates, isotopic labeling, cross-over experiment and stereo chemical evidence.

Linear Free Energy Relationship: Hammett equation, physical significance of  $\sigma$  and  $\rho$ , applications and limitations. Taft equation.

### Reference Books:

1. Eliel, E.L., & Wilen, S.H. (2003). Stereochemistry of organic compounds. John Wiley and sons Inc.
2. Nasipuri, D. (1991). Stereochemistry of Organic Compounds - Principles and Applications. Wiley Eastern, Ltd.
3. Carey, F.A. (2005). Organic Chemistry. Tata McGraw Hill.
4. March, J. (2006). Advanced Organic Chemistry. (4<sup>th</sup> ed.), John Wiley and Sons, New York.
5. Morrison, R.T., & Boyd, R.N. (1997). Organic Chemistry. Prentice Hall.
6. Ferguson, L.N. (1966). The Modern Structural Theory of Organic Chemistry. Prentice Hall.
7. Pine, S.H., Hendrickson, J.B., Cram, C.J., & Hammond, G.S. (1980). Organic Chemistry. (4<sup>th</sup> ed.), McGraw Hill, Kogakusha Ltd.
8. Norman, R.O.C. (1993). Principles of Organic Synthesis, Chapman Hall, London.
9. Bansal, R.K. (2005). Reaction Mechanism in Organic Chemistry. (3<sup>rd</sup> ed.), Tata McGraw Hill,
10. Finar, I.L. (2001). Organic Chemistry. (5<sup>th</sup> ed.), Vol. I and II. ELBS
11. Eliel, E.L. (1999). Stereochemistry of Carbon Compounds. Mc Craw Hill.
12. Kalsi, P.S., (2000). Stereo chemistry Conformation and Mechanism. New Age International, Ltd.
13. Ahluwalia, V.K., & Parshar, R.K. (2005). Organic Reaction Mechanism. (2<sup>nd</sup> ed.), Narosa publishing House
14. Sykes, P. A. (2003). Guide Book to Mechanism in Organic Chemistry. Orient Longman.

## Inorganic Chemistry I

Sub. Code: PG1712

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

### Objectives:

1. To provide a firm foundation on transition elements.
2. To gain knowledge on co-ordination complexes and its reactions.
3. To know the importance of organometallic compounds.
4. To understand properties and theories related to solids.
5. To learn the preparation, properties and structures of some Inorganic compounds.

## **Unit I: Chemistry of transition elements**

Second and third series: Zirconium and Hafnium- Occurrence, isolation and oxidation states. Aqueous Chemistry -  $Zr^{4+}$  and  $Hf^{4+}$ - halides,  $ZrO_2$  and mixed oxides, Zr clusters. Niobium and Tantalum - Occurrence, isolation, oxidation states, oxygen compounds, fluorides – pentafluoride.

Rhenium- Occurrence, isolation and oxidation states. Rhenium heptafluoride-  $ReCl_5$ ,  $ReCl_4$  and Re III chlorides.

General characteristics of Ruthenium and Osmium: Nitrogen - Ligand complexes of Ru. Creutz- Taube and related complexes - Rh and Ir- Wilkinson's catalyst -Pt complexes in the treatment of cancer. Preparation and properties of  $UF_4$ ,  $UO_2(NO_3)_2 \cdot 9H_2O$ ,  $ThO_2$ ,  $Th(NO_3)_2$ ,  $PtCl_4$ ,  $H_2PtCl_6$  and  $Cis-PtCl_2(NH_3)_2$

## **Unit II: Co-ordination Chemistry**

Stability constant, Determination of stability constant by Jobs and spectrophotometric methods. Magnetic and spectral properties of complexes  $[Ti(H_2O)_6]^{3+}$  and  $[Cu(H_2O)_6]^{2+}$ . Chelate compounds. Nephelauxetic effect.

Substitution in octahedral complexes. Acid hydrolysis. Base hydrolysis. Electron transfer reactions - Outer sphere and inner sphere mechanism. Applications of electron transfer reactions in synthesis of coordination complexes. Mechanism of ascorbic acid oxidation by free and chelate Cu(II) Complexes.

## **Unit III: Organometallic Chemistry**

Introduction, EAN and its correlation to stability. Synthesis and structures of metal carbonyls. Carbonylate anions. Carbonyl hydride complexes and metal nitrosyls. Isolobal analogy. IR study of metal carbonyls.

Synthesis, properties and structural features of metal complexes with carbene, alkene, alkyne and arene. Hapticity. Metallocenes - Synthesis, properties and bonding in ferrocene. Covalent versus ionic bonding in zirconocene.

## **Unit IV: Solid State**

Electronic structure of solids - Free electron and band theory type of solids -conductors, insulators, intrinsic and extrinsic semiconductors.

Optical and electrical properties of semiconductors- photovoltaic effect, Hall effect. Metal-metal and metal-semiconductor junction. Superconductivity - high temperature superconductors, properties and applications. BCS theory, Cooper electrons, Meissner effect and levitation. Crystal defects in solids - line and plane defects. Colourcentres. Solid electrolytes and their applications.

## **Unit V: Inorganic chains, Rings, Cages and Clusters**

Silicates: classification- soluble and insoluble, based on  $(SiO_4)^{4-}$  linkage -ortho, pyro, cyclic, chain, sheet, three-dimensional silicates - Intercalation chemistry of silica and graphite - Polyacids-structure of isopoly and heteropoly anions, Polythiazyl- preparation and properties - Borazines- preparation, similarity with benzene and applications - Phosphazenes- preparation and structure- Craig and Paddock, Dewar's model - Preparation of carboranes, Diborane- preparation, structure and chemical properties, preparation and structure of tetraborane, structures of pentaborane-9, pentaborane-11, hexaborane-10 and decaborane-14 -

Metal clusters: Carbonyl type - structure of four, five and six atom clusters - Anionic and hydrido clusters, Non carbonyl type - Octahedral and triangular clusters.

**Reference Books:**

1. Cotton, F.A., & Wilkinson, G. (1970). Advance Inorganic Chemistry. (2<sup>nd</sup> ed.), Wiley Eastern Private Ltd.
2. Soni, P.L. (1991). A text book of Inorganic Chemistry, Sultan Chand Sons Publishers.
3. Puri B.R., Sharma, L.R., & Kalia, K.C. (2012). Principles of Inorganic Chemistry. (4<sup>th</sup> ed.), Milestone publishers.
4. West, A.R. (1998). Solid State Chemistry and its Application, John Wiley & Sons, Asia.
5. Kittle, C. (1993). Introduction to Solid State Physics, Wiley Eastern Ltd.
6. Douglas, B.E., McDaniel, D.H., & Alexander, J.J. (1983). Concepts and Models of Inorganic Chemistry. (2<sup>nd</sup> ed.), John Wiley and Sons Ltd.
7. Miessler, G.L. (2004). Inorganic Chemistry. (3<sup>rd</sup> ed.), Pearson Education Inc.
8. Bannerje, D. (1993). Coordination Chemistry, Tata McGraw Hill.

**Physical Chemistry I**  
**Sub. Code: PG1713**

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

**Objectives:**

1. To know about Thermodynamics and Phase Rule.
2. To learn the various concepts and equations related to Statistical Thermodynamics.
3. To study the kinetics of reactions.
4. To gain more knowledge about Quantum Mechanics.
5. To acquire knowledge about surfaces and surface active agents.

**Unit I: Thermodynamics and phase rule**

Thermodynamics: Partial molar properties- Significance and determination by intercept and density methods, Partial molar free energy - Gibb's-Duhem equation, Definitions for Chemical potential, Partial molar volume and partial molar heat content- variation of chemical potential with temperature and pressure. Choice of standard states- components in gases and solution. Determination of activity and activity coefficients for non-electrolytes.

Phase rule: Definitions of phase and components, three liquid components forming one, two or three pairs of partially miscible liquids.

Two solids and water systems involving (i) no chemical combination (ii) forming of a double salts- decomposed and not decomposed by water (iii) formation of a hydrate- dehydrated and not dehydrated by second salt and by one salt.

**Unit II: Statistical thermodynamics**

Aim, permutation and combinations. Thermodynamic probability and entropy. Ensemble - canonical and microcanonical and grand canonical. Maxwell-Boltzmann statistics, Bose-Einstein statistics and Fermi-Dirac statistics. Population inversion, negative Kelvin temperature. Comparison of MB, BE and FD.

Derivation of distribution laws-Partition function-translation, rotational, vibrational and electronic partition function. Thermodynamic functions in terms of partition function-internal energy and entropy. Relationships between partition function and work, pressure, enthalpy, Gibbs free energy and internal energy. Sacker-Tetrode equation.

### **.Unit III: Chemical kinetics - I**

Arrhenius equation. Simple collision theory. ARRT theory-statistical and thermodynamic treatments. Ionic reactions - primary and secondary salt effects. Derivation and significance of volume of activation.

Kinetic isotopic effect, Kinetics of unimolecular reaction-Lindemann, Hinshelwood and Rice-Ramsperger-Kassel Marcus.

Fast reactions- General features - flow techniques - relaxation theory and relaxation techniques (T-jump and p jump) - crossed molecular beam technique.

### **Unit IV: Quantum mechanics - I**

Quantum mechanical operators: Addition, subtraction and multiplication of operators, position operator, linear operators, linear momentum operator, angular momentum operator, kinetic energy operator and Hamiltonian operator, Hermitian operator-commutation relationship among  $L_x$ ,  $L_y$ ,  $L_z$  and  $L^2$  operators.

Wave functions, Eigen functions and eigen values-orthogonality and normalization. Schrodinger time independent wave equation, De-Broglie equation, Heisenberg's uncertainty principle, postulates of quantum mechanics, setting up of schrodinger equation, solution and interpretation with regard of particle in 1 D box, particles in a 3D box, simple harmonic oscillator.

### **Unit V: Surface chemistry**

Electrical aspects of surface chemistry, electrical double layer, Zeta potential. BET and Gibbs adsorption isotherms- Derivation and application. Determination of surface area (BET equation) surface films and liquids. Membrane equilibria and dialysis.

Surface active reagents: Classification of surface agents-micellization, hydrophilic interactions-critical micellar concentration-factors affecting the CMC of surfaces. Adsorption on semiconductor surfaces. Transition state theory of surface reactions - rates of chemisorptions - Hertz-Knudson equation.

### **Reference Books:**

1. Glasstone, S. (1969). Thermodynamics for chemistry, Van Nostrand Co, New York.
2. Glastone, S.A. (1969). Text Book of Physical Chemistry. (2<sup>nd</sup> ed.), Macmillan and Co Ltd
3. Kuriacose, J.C., & Rajaram, J. (1986). Thermodynamics. Shohanlal and Co. Delhi.
4. Laidler, K.J. (1987). Chemical Kinetics. (3<sup>rd</sup> ed.), Harper and Row, New York.
5. Chandra. A.K. (2001). Introductory Quantum Chemistry. (4<sup>th</sup> ed.), Tata McGraw-Hill.
6. Barrow, G.M. (1988). Physical Chemistry, McGraw Hill.
7. Maron, S.H., & Prutton, C.F. (1965). Principles of Physical Chemistry. (4<sup>th</sup> ed.), Oxford& IBH publishing Co. Pvt. Ltd.
8. Kapoor, K.L. (1986). Text Book of Physical Chemistry. MacMillan India Ltd, Delhi.
9. Atkins, P., & Atkins, J.P. (2002). Physical Chemistry. (7<sup>th</sup> ed.), Oxford university press.
- Gowariker, V.R. (2000). Polymer Science, Wiley Eastern Ltd.

**Semester I**  
**Instrumental Methods of Analysis (Elective I)**  
**Sub. Code: PG1714**

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

**Objectives:**

1. To gain knowledge about different chromatographic techniques and its applications
2. To know the principles involved in chromatographic techniques
3. To learn the principles, instrumentation and applications of TGA and DTA.
4. To study the principles and applications of spectrophotometric analytical techniques.
5. To understand the principles and instrumentations of spectroscopy techniques.

**Unit I: Chromatography I**

Chromatography: Definition, plate and rate theories and classification. Paper chromatography - Principle. Types - ascending, descending and radial paper chromatography, applications.

Thin layer chromatography - experimental technique and applications. Column chromatography- principle, experimental technique and applications.

**Unit II: Chromatography II**

Ion exchange chromatography: Principle, experimental techniques, applications, separation of zinc and magnesium, chloride and bromide.

High performance liquid chromatography: Principle, experimental technique and applications.

Gas chromatography: Principle, experimental technique and applications.

**Unit III: Thermo Analytical and Electroanalytical Methods**

Thermogravimetric analysis (TGA) - principle, automatic thermogravimetric analysis, factors affecting TGA, applications. Thermometric titrations. Differential thermal analysis (DTA), simultaneous DTA, TGA curves.

Electrogravimetric analysis - theory, instrumentation, applications. Coulometric analysis -coulometric titrations, applications. Potentiostaticcoulometry.

Polarography: Principle, dropping mercury electrode, experimental assembly, polarographic curves, applications to qualitative and quantitative analysis, concept of pulse polarography. Amperometric titrations -principles and applications.

**Unit IV: Colorimetric and Spectrophotometric Analysis**

Colorimetry - Instrumentation for visual colorimetry, photoelectric colorimetry. Spectrophotometry - Instrumentation. Fluorometry - principle, instrumentation, applications. Flame photometry- principle, instrumentation and application. Nephelometry and turbidimetry- theory and instrumentation, turbidimetric titrations and applications.

**Unit V: Spectroscopy**

Principles and Instrumentation techniques of UV, IR, Raman, <sup>1</sup>HNMR, Mass, Mossbauer and AAS.

**Reference Books:**

1. Kaur, H. (2007). An Introduction to Chromatography. (2<sup>nd</sup> ed.) Pragati Prakashan Publishing Ltd.
2. Higson, S. (2003). Analytical Chemistry. (1<sup>st</sup> ed.), Oxford University Press, USA,

- Kaur, H. (2014). Instrumental Methods of Chemical Analysis. Pragati Prakashan Publishing Ltd.
- Mohan, J. (2001). Organic Spectroscopy Principles and Applications. Narosa publishing house.
- Christian, G.D. (2007). Analytical Chemistry. (6<sup>th</sup> ed.), John Wiley & Sons.
- Cases, M.V. (2000). Principles of Analytical Chemistry. A Textbook, Springer.
- Chatwal, G.R., & Anand, S.K. (2002). Instrumental Methods of Chemical Analysis. (5<sup>th</sup> ed.), Himalaya Publishing House.
- Day, R.A., & Underwood, A.L. (1998). Quantitative Analysis. (6<sup>th</sup> ed.), Prentice Hall of India.
- Kemp, W. (1994). Organic Spectroscopy. (3<sup>rd</sup> ed.), Macmillan.
- Silverstein, S.M., Bassler, G.V., & Morrill, T.C. (2004). Spectrometric Identification of Organic Compounds. (6<sup>th</sup> ed.), Wiley.

**Semester I**  
**Electrochemistry (Elective I)**  
**Sub. Code: PG1714**

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

**Objectives:**

- To acquire knowledge about industrial electrochemistry.
- To gain knowledge about the applications of electrochemistry in metallurgy.
- To study the uses of electro and electro less plating.
- To know the types of batteries and cells.
- To understand the types of corrosion and methods of prevention of corrosion.

**Unit I: Industrial Electrochemistry**

Electrochemical processes in industry - components of electrochemical reactors - Types of electrolytes - Cathodes and anodes in electrochemical reactor - Separators.

Electro Inorganic Chemicals - Caustic soda and chlorine production, mercury cells, diaphragm cells, membrane cells, Advantages of membrane cells - Other inorganic electrochemicals - Chlorates, perchlorates, hydrogen peroxide.

Organic Electrochemicals - Special features of electro- organic synthesis - electrochemical oxidation- Kolbe synthesis -Electroreduction of carbonyl compounds - Adiponitrile synthesis.

**Unit II: Electrometallurgy**

Electrodeposition of metals - principles - Nucleation and growth of crystals - Nature of electrodeposits.

Hydrometallurgy- Recovery of metals from aqueous electrolytes - Recovery of silver from photographic emulsion -Electrorefining- Production of high purity copper - Process description.

Pyrometallurgy- Necessity for using molten electrolytes - Reactors for molten salt electrolysis- Production of Aluminium- Electrodes and electrode reactions in cryolite melt-electrochemical purification of Aluminium- Other metals through molten salt electrolysis - Mg and Na - Brief outline.



### Unit III: Electroplating

Fundamental principles – Nature of deposits for electroplating – Hull cell experiments – operating conditions and nature of deposits – throwing power – preparation of samples for electroplating – chemical and electrochemical cleaning – electroplating of copper, nickel and cadmium.

Electroless plating– Importance – plating on nonmetals – Bath composition – Electroless plating of copper and nickel.

### Unit IV: Electrochemical power sources

Basic principles – chemical and electrical energies – Interconversion – charging and discharging – requirements for a good power source – types of power sources.

Primary batteries – Description of primary cells – Alkaline – Manganese cells – Button cells – Silver oxide – Zinc cells- Lithium primary cells – Applications.

Secondary batteries: Important applications – Charge discharge efficiency – Cycle life – Energy density – Lead acid batteries – Nickel – metal hydride batteries – Lithium – secondary batteries – Batteries for electrical vehicles.

Fuel cells:Basic principles – H<sub>2</sub>, O<sub>2</sub> fuel cells – gas diffusion electrodes for fuel cells – Alkaline fuel cells only.

### Unit V: Corrosion

Principles – stability of metals – EMF series – Active and noble metals – PH effect on stability – Pourbaix diagram – Kinetics of corrosion – Mixed potential process –Cathodic reaction – Anodic reaction – corrosion current – Active dissolution – passivation – Breakdown of passivity- Evans diagram.

Methods of corrosion protection: Principles – Inhibition of anodic,cathodic processes – Inhibitive additives for corrosion protection – Protective coatings – Types of coatings – Protection of structures and pipelines – Cathodic Protection – Examples – Sacrificial anodes – protection of ships in sea water.

### Reference books:

1. Hamann, C.H., Hamnett, A., & Vielstich, W. (2001). Electrochemistry. (4<sup>th</sup> ed.), John Wiley and Sons, New York.
2. Hibbert, D.B. (1981). Introduction to Electrochemistry. Macmillan, London.
3. Pletcher, D., & Walsh. F.C. (1993). Industrial Chemistry. (3<sup>rd</sup> ed.), Blackie Academic and Professional, London.

**Semester I**  
**Practical I**  
**Organic Chemistry**  
**Sub. Code: PG17P1**

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

### Objectives

1. To provide knowledge about the separation of binary mixtures.
2. To gain skill in analyzing the functional groups.
3. To estimate various organic substances.
4. To prepare organic compounds.

### 1. Separation of a Binary mixture (Minimum six binary mixtures)

Quantitative chemical separation of a binary mixture following a systematic procedure. The two components should not interact at room temperature. They should be sufficiently soluble in ether. Two neutral components should be avoided. A few possible combinations are:

- a. Any acidic component and a neutral substance
- b. Any basic component and a neutral substance
- c. A carboxylic acid and a phenol
- d. A phenol and a basic component

The two components must be exhibited along with weight, in the normal physical state of the substance.

### 2. A quantitative estimation of any one of the following in an organic substance. (Minimum five estimations)

- a. Glucose- Lane and Eynon method
- b. Glucose- Bertrand's method
- c. Estimation of phenol
- d. Estimation of aniline
- e. Iodine value of an oil
- f. Number of hydroxyl groups in a given compound.
- g. Estimation of Ethyl methyl ketone

### 3. Preparation of a solid compound involving a familiar name reaction – rearrangement in two stages. (Minimum five preparations)

- a. P-Bromoaniline from Acetanilide
- b. P-Nitroaniline from acetanilide
- c. Benzpinacolone to Benzophenone
- d. Benzaniilide from Benzophenone
- e. S-Benzylisothiuroniumbenzoate from Thiourea
- f. S-Tribromobenzene from Aniline.
- g. Phthalimide from phthalic acid.

Students are expected to submit five recrystallised samples of the final products at the time of practical examination for evaluation by the examiners.

### Reference Books

1. Dey, B.B., Sitaraman M.V. & T.R. Govindachari. (1992). Laboratory Manual of Organic Chemistry. (2<sup>nd</sup> ed.), Allied Publishers, New Delhi.
2. Vogel, A.I. (1987). Quantitative Organic Analysis Part III. (2<sup>nd</sup> ed.), CBS Publishers, New Delhi.

**Semester II**  
**Organic Chemistry II**  
**Sub. Code: PG1721**

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

**Objectives**

1. To study the nucleophilic substitution and elimination reactions
2. To know about Huckel's rule, antiaromaticity and homoaromaticity
3. To learn name reactions in organic chemistry.
4. To gain knowledge on bio-active molecules and its functions.
5. To understand the structure and synthesis of natural products.

**Unit I: Substitution and Elimination Reactions**

Aliphatic nucleophilic substitution:  $S_N^1$ ,  $S_N^2$ ,  $S_N^i$  mechanism. Effect of substrate, nucleophile, leaving group and solvent on aliphatic nucleophilic substitution.  $S_N^1$ ,  $S_N^2$  and  $S_N^i$  mechanism for allylic system. Aromatic nucleophilic substitution -  $S_N^{Ar}$ ,  $S_N^1$  and  $S_N^2$ . Effect of substrate, structure, nucleophile, leaving group and solvent on aromatic nucleophilic substitution. Ortho-, para- and meta- directing groups in aromatic nucleophilic substitution. Neighbouring group participation of alkyl and aryl groups, halogens, carboxylate anion, oxygen, sulphur, C=C bond and C-C bond. Elimination -  $E_1$ ,  $E_2$  and  $E_{1CB}$  mechanisms. Effect of substrate, base, solvent and the leaving group on elimination reaction. Hofmann, Saytzeff and Bredt's rule.

**Unit II: Aromaticity and Novel Ring System**

Aromaticity: Huckel's rule, five, six, seven and eight membered rings, fused six membered aromatic rings. Aromaticity of fulvene, fulvalene, azulene, tropolones, ferrocene and fullerenes. Non-benzenoid aromatics - annulenes, heterocyclic compounds. Craig's rule of aromaticity. Concept of antiaromaticity and homoaromaticity. Calculation of energy of aromatic and anti-aromatic systems. Alternant and non-alternant hydrocarbons.

Novel ring system: Nomenclature of bicyclic and tricyclic systems – structure and synthesis of adamantane, congressane, cubane and catanene.

**Unit III: Organic name reactions**

Mechanism and applications: Sharpless asymmetric epoxidation, Stobbe condensation, Dieckman condensation, Robinson annulations, Oppenauer oxidation, Meerwein-Ponndorf Verley reduction, Wolf-Kishner reduction, Clemmensen reduction and Birch reductions, Simon-Smith, Bischler-Napieralski, Chichibabin, Ziegler alkylation and Vilsmeier-Heck reactions.

**Unit IV: Chemistry of bio-active molecules**

Proteins: primary structure of proteins, terminal group analysis, Edman degradation and DNP method. Secondary structure of protein principles leading to  $\alpha$  –helix and  $\beta$  sheet structure. Tertiary and quaternary structures. Structural elucidation of oxytocin - Tuppy's method (Synthesis not required) and insulin (Biosynthesis). Polynucleotides and polynucleosides, role and function of RNA's in protein synthesis, DNA replication, transcription and translation.

Lipoproteins: LDL, HDL and their characteristics.

Antibiotics: Structural activity relationship of penicillins, cephalosporin, streptomycin and chloramphenicol.

## Unit V: Natural Products

Steroids: Structural elucidation of cholesterol (Synthesis not required), bile acids - Lithocholic acid.

Sex-hormones: Synthesis of Progesterone, oestrone, oestriol, oesterodiol, testosterone and androsterone. Conversion of cholesterol into androsterone, Progesterone and testosterone. Conversion of oestrone into oestriol, oesterodiol.

## Reference Books

1. March, J. (2006). Advanced organic chemistry. (4<sup>th</sup> ed.), John Wiley and Sons, New York.
2. Finar, I.L. (2001). Organic Chemistry. (5<sup>th</sup> ed.), Vol. I and II, ELBS.
3. Clayden, J., Greeves, N., & Warren. S. (2012). Organic Chemistry, Oxford University Press.
4. Kar, A. (2006). Medicinal Chemistry. (4<sup>th</sup> ed.), New Age international Ltd.
5. Agarwal, O.P. (1984). Chemistry of Natural Products. Vol. I and II, Goel publishing House, Meerut.
6. Chatwal, G. (1992). Organic Chemistry of Natural Products. Vol. I and II, Himalaya Publishing House, Bombay.
7. Ahluwalia, V.K., & Parshar, R.K. (2005). Organic Reaction Mechanism. (2<sup>nd</sup> ed.), Narosa, publishing House.
8. House, H.O. (1972). Modern Synthetic Reaction. (2<sup>nd</sup> ed.), W.A. Benjamin, Inc., London.
9. Solomons, T.W.G. (2009). Organic Chemistry. Craig Fryhle Wiley.
10. Ghosh, J. (2014). A Textbook of Pharmaceutical Chemistry. S. Chand & Company Ltd.

## Semester II Inorganic Chemistry II Sub. Code: PG1722

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

## Objectives

1. To provide an in-depth knowledge about lanthanides and actinides.
2. To understand the photochemistry of some Inorganic compounds.
3. To enable the students gain knowledge about the role of Inorganic compounds in life.
4. To get clear information about I.R and Raman spectroscopy.
5. To understand the techniques for the study of Inorganic compounds.

## Unit I: Lanthanides and Actinides

Lanthanides and actinides: Correlation of electronic structures, occurrence and properties of the elements. Chemistry of separation of Np, Pu and Am from U fission products. Common and uncommon oxidation states. Lanthanide and actinide contractions. Spectral and magnetic properties of lanthanides and actinides, similarities between actinides and lanthanides.

Preparation and properties of  $UF_4$ ,  $UO_2(NO_3)_2 \cdot 9H_2O$ ,  $ThO_2$ ,  $Th(NO_3)_2$ .

## Unit II: Inorganic Photochemistry

Importance of photochemistry. Photochemistry of Co(III) complexes - photosubstitution reactions, photooxidation-reduction reactions (redox), photoanation reactions.

Photochemistry of Cr(III) complexes : Photoaquation – octahedral complexes, mixed-ligand complexes, photoisomerization, photoracemization, photoanation, photosubstitution in non-aqueous solvents, photoredox reactions.

Photochemistry of Ruthenium polypyridyls: Preparation of  $[\text{Ru}(\text{bpy})_3]^{2+}$ , important characteristics of  $[\text{Ru}(\text{bpy})_3]^{2+}$ , properties of  $[\text{Ru}(\text{bpy})_3]^{2+}$ - absorption spectroscopy, ground state properties, redox properties, emission spectroscopy, photosubstitution reaction, photo redox reaction and reductive quenching.

### **Unit III: Bio Inorganic Chemistry - I**

Metalloporphyrins, porphyrin ring in chlorophyll. Photosynthetic electron transport sequence. Biological electron transfer. Electron transfer agents - cytochromes, iron-sulphur proteins. Blue Copper proteins - Stenocyanin, Plastocyanin, Azurin, Non-blue copper proteins. Synthetic oxygen carriers. Vitamin B<sub>1</sub>, B<sub>2</sub>, B<sub>6</sub> and Vitamin B<sub>12</sub> coenzymes. Nitrogen fixation - invitro and invivo nitrogen fixation. Chelate therapy-therapeutic chelating agents and their uses- anticancer platinum complexes and their interaction with DNA.

### **Unit IV: Application of spectroscopy to the study of inorganic compounds - I**

IR and Raman Spectroscopy: Application of IR and Raman spectra in the study of coordination compounds. Application to metal carbonyls and nitrosyls. Geometrical and linkage isomerism. Detection of inter and intramolecular hydrogen bonding. Stretching mode analysis of metal carbonyls.

Photoelectron Spectroscopy: Basic principles, Koopmans's theorem. UPS, XPEs of N<sub>2</sub>, O<sub>2</sub> and NH<sub>3</sub>-chemical shifts in XPES. Application of ESCA to inorganic systems-Auger electron spectroscopy.

### **Unit V: Applications of spectroscopy to the study of inorganic compounds - II**

Electronic spectra: Term, states and microstates, term symbols, selection rules, Hund's rule, LS coupling, J - J coupling schemes, Racah parameters B and C. Orgel and Tanabe-Sugano diagrams - Evaluation of 10 Dq and  $\beta$  for octahedral Ni<sup>2+</sup> system, tetrahedral Co<sup>2+</sup> complexes. Charge transfer spectra - Applications of charge transfer spectra. Electronic spectra of lanthanide and actinide complexes.

### **Reference Books**

1. Huheey, J.E., Keiter, E.A., Keiter, R.L., & Medhi, O.K. (2011). Inorganic Chemistry, Principles of Structure and Reactivity. (4<sup>th</sup> ed.), Pearson Education.
2. Lee, J.D. (2008). Concise Inorganic Chemistry. (5<sup>th</sup> ed.), Wiley India.
3. Malik, W.U., Tuli, G.D., & Madan, R.D. (2012). Selected topics in Inorganic Chemistry. S. Chand Company Ltd.
4. Glasstone, S. (1969). Source Book of Atomic Energy. East West Pvt. Ltd.
5. Chatwal, G.R., & Bhagi, A.K. (2005). Bio-inorganic Chemistry. (2<sup>nd</sup> ed.) Himalaya Publishing House.
6. Rohatgi, K.K., & Mukherjee, K.K. (2014). Fundamentals of Photochemistry. (3<sup>rd</sup> ed.), New Age International.
7. Cotton, F.A., Wilkinson, G., Marilo, C.A., & Bochman, M. (1999). Advanced Inorganic Chemistry. (6<sup>th</sup> ed.), Wiley Interscience Publication.
8. Manku, G.S. (2004). Theoretical Principles of Inorganic Chemistry. Tata McGraw Hill.
9. Douglas, B.E., Mc Daniel D.H., & Alexander, J.J. (1983). Concepts and Models of Inorganic Chemistry. (2<sup>nd</sup> ed.), John Wiley and Sons Ltd.

10. Shriver, D.F., & Atkins, P.W. (1994). Inorganic Chemistry. ELBS, Oxford University Press.

**Semester II**  
**Physical Chemistry II**  
**Subject code: PG1723**

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

**Objectives**

1. To study about the theories of electrical conductance.
2. To understand the concepts of electrochemistry and know corrosion.
3. To study the process of photochemical reactions.
4. To learn about homogenous and heterogeneous catalysis.
5. To understand Quantum Mechanics and apply to various molecules.

**Unit I: Electrochemistry - I**

Debye Huckel limiting law, determination of activity coefficient by electrical method, Debye-Huckel limiting law at appreciable concentration of electrolytes, Huckel equation, Debye Huckel Bronsted equation - qualitative and quantitative verification. Electrode-electrolyte interface, electrolytic interface, adsorption at electrified interface-alloy deposition, electrical double layer, electro capillary phenomenon- Lippmann equation.

**Unit II: Electrochemistry - II**

Electrode potential, mechanism of electrode reaction polarization and over potential-theory and applications of over potential, Butler-Volmer equation, electron transfer reaction. Significance of electron exchange current density and symmetry factor. Transfer coefficient and its significance. Mechanism of hydrogen and oxygen evolution reactions.

Corrosion- corrosion of common metals, atmospheric and immersed types of corrosion, acid, colloidal, oxide-film, electrochemical and differential aeration theories, passivation of metals- Pourbaix diagram, Evan's diagram. Fuel cells, acid and alkaline storage batteries, Electrode deposition-principle and applications.

**Unit III: Photochemistry**

Introduction to photochemistry- laws of photochemistry, quantum yield calculation, physical properties of electronically excited molecules ,excited state dipolemoment, acidity constant and redoxpotential-photophysical processes in electronically excited molecules, Jablonski diagram-intersystem crossing -internal conversion, fluorescence, phosphorescence and other deactivation processes - Delayed fluorescence-Stern-Volmer equation and its application. Photosensitization and chemiluminescence. Chemical lasers - photoexplosion and dissociation laser-experimental techniques-chemical actinometry and flash photolysis.

**Unit IV: Catalysis**

Homogenous Catalysis: General catalytic mechanism (equilibrium treatment and steady state treatment) - general acid - base catalysis and determination of catalytic co-efficient discussion of protolytic and prototropic mechanisms of acid catalysis. Bronsted relationships as linear free energy relationships. Acidity functions and correlation of mechanisms.

Heterogeneous Catalysis: Physisorption and chemisorption - Langmuir adsorption isotherm, mechanism of surface reactions (Langmuir - Hinshelwood and Eley Rideal mechanism), absolute rate of surface reactions.

### Unit V: Quantum mechanics - II

Approximation methods - Variation Theorem- Application of variation principle to Helium atom. Perturbation theory – application of perturbation theory to Helium atom. Pauli's exclusion principle – Secular determinant and secular equation , Slater determinant.

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

Chemical bonding in diatomic molecules - Born Oppenheimer approximation –M.O. theory. LCAO approximation – application to hydrogen molecule ion  $H_2^+$ – Hydrogen molecule  $H_2$ , Valence bond theory, application to  $H_2$  molecule.

### Reference Books

1. Glasstone, S. (1965). An Introduction to Electrochemistry, Van Nostrand. New York.
2. Glasstone, S. (1969). A Text Book of Physical Chemistry. (2<sup>nd</sup> ed.), Macmillan and Co Ltd.
3. Rohatgi-Mukherjee, K.K. (1997). Fundamentals of Photochemistry. New Age International (P) Ltd.
4. Chandra, A.K. (2001). Introductory Quantum Chemistry. (4<sup>th</sup> ed.), Tata McGraw-Hill.
5. Laidler, K.J. (2004). Chemical Kinetics. (3<sup>rd</sup> ed.), Pearson Education.
6. Bradley, J.N. (1975). Fast Reactions. Clarendon Press, Oxford.
7. Mortimer, R.G. (2008). Physical Chemistry. Academic Press.
8. Atkins, P.W. (2009). Physical Chemistry. (9<sup>th</sup> Ed.), Oxford University Press.

## Semester II Research Methodology Elective II Sub. Code: PG1724

### Objectives

1. To motivate the students for research based studies.
2. To gain knowledge about statistical analysis.
3. To enrich them with wide knowledge of instrumentational analysis.
4. To get a basic idea related to the application of computers in research.
5. To gain basic knowledge on cheminformatics.

### Unit I: Literature Searching and Preparation of Project Report

Sources of information: primary, secondary and tertiary sources - Libraries, Databases, Abstracts, Journals, Books, Newspapers, Government documents, Conference proceedings, Dissertations and thesis. Internet - Inlib net. Presentation of seminar - OHP and power point. Project report writing - International conventions.

### Unit II: Statistical Analysis

Classification of errors. Expression and calculation of errors in different forms - Precision and accuracy with respect to random errors. Confidence limits. Tests of significance - F-test, t-test, chi square test and annova. Regression analysis - correlation analysis.

### Unit III: Instrumental Analysis

Applications of UV, IR, NMR, and Mass spectra in structural elucidations. ESR, Study of morphology – Principle of XRD and SEM, STM and AFM and application.

### Unit IV: Computer in Research

Basic features common to Word, Excel, Access, Powerpoint. Toolbars, dialog box, Internet: introduction, history, types of internet connections, HTML, HTTP, web design, hyperlinks, URLS, domain server, static and dynamic ID, protocols and internet security.

### Unit V: Cheminformatics

Cheminformatics: History, Representing molecules: older systems - connection tables, line notation – Inchi, SMILES, WLN canonicalization. Line notation versus connection tables. Query languages – SMARTS. Nomenclature: IUPAC names, trade names, common names. Molecular similarity: Ways to measure similarity – 2D topology, 3D configuration, Physical properties, clustering. Chemical registration system. Chemistry softwares.

### Reference Books

1. Berg, B.L. (2009). Qualitative Research Methods for the Social Sciences. (7<sup>th</sup> ed.), Pearson Education Inc.
2. Patton, M.Q. (2002). Qualitative research and evaluation methods. (3<sup>rd</sup> ed.), Sage Publications.
3. Silverman, D. (2011). Qualitative Research: Issues of Theory, Method and Practice. (3<sup>rd</sup> ed.), Sage Publications.
4. Polanski, J. (2009). Chemoinformatics, Elsevier Publications.
5. Marczyk, G., Dematteo, D., & Festinger, D. (2005). Essential of Research Design and Methodology. John Wiley & Sons, Inc.
6. Vogel, A.I. (1978). A Text Book of Quantitative Inorganic Analysis. (4<sup>th</sup> ed.), ELBS.
7. Maidasane, D. (2005). Learning Computer Fundamentals, MS Office and Internet and Web Technology. Firewall media, New Delhi.
8. Gasteiger, J., & Engel, T. (2003). Chemoinformatics, Wiley, New York.

### Semester II

#### Nuclear Chemistry (Elective II)

Sub. Code: PG1724

Gravimetric analysis and Inorganic preparations

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

### Objectives

1. To provide knowledge about the radioactivity and its measurement.
2. To learn the types of nuclear reactions and their mechanisms.
3. To know the types of nuclear reactors and the fuels used in them.
4. To understand the interaction between radiation and matter.
5. To gain knowledge on applications of radio isotopes in industries and daily life.

### Unit I: Radioactivity and its Measurement

Discovery - types of decay - decay kinetics - half-life period, mean life, parent-daughter 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, semiconductor detectors, thermoluminescence detectors and neutron detectors.

### Unit II: Nuclear Reactions

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: Nuclear Reactors

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 - Nuclear waste management - safety culture - active and passive safety. Containment building, nuclear criticality safety, ionizing radiation protection - enforcement agencies.

### Unit IV: Radiation and Matter

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: Applications of Radioactivity

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 - Use of nuclear reactions - Radioisotopes as source of electricity - Nuclear medicines.

### Reference Books

1. Glasstone, S. (1967). Source Book on Atomic Energy. (3<sup>rd</sup>ed.), East West press.
2. Arniker, H.J. (2009). Essentials of Nuclear Chemistry. New age International.
3. Friedlander, M.G., Kennedy, J.M., E.S. Macian & J.M. Miller. (1981). Nuclear and Radiochemistry. (3<sup>rd</sup> ed.), John Wiley and Sons.
4. Arora M.G. & Singh, M. (1994). Nuclear Chemistry, Anmol Publications.
5. Gilreath, E.S. (1982). Fundamental Concepts of Inorganic Chemistry. McGraw Hill

**Semester II**  
**Practical II**  
**Inorganic Chemistry**  
**Sub. Code: PG17P2**

No. of hours per week	Credit	Total no. of hours	Marks
6	5	90	100

### Objectives

1. To gain knowledge in Semi micro qualitative analysis of inorganic mixture.
2. To impart skill in estimating the presence of various elements.

- To estimate the elements by Photocolorimetric method.
  - To identify inorganic cations in a binary mixture.
- Semi micro qualitative analysis of inorganic mixture containing two familiar and two less familiar cations.  
Pb, Cu, Bi, Cd, Sb, Zn, Co, Ni, Mn, Ca, Ba, Sr, W, Ti, Se, Te, Mo, Ce, Th, Zr, V, U, Ti and Li.
  - Complexometric titration – Estimation of Cu, Zn and Mg by EDTA titration in presence of either Pb or Ba.
  - Photocolorimetric estimation of Fe, Ni, Cr, Mn, Cu and  $\text{NH}_4^+$
  - Separation and identification of a binary mixture of inorganic cations by paper chromatography.

### Reference Books

- Davies D.G. & Kelly, T.V.G. (1969). Inorganic Reactions at Advanced Level, Mills and Boom publications.

**SEMESTER – III**  
**ORGANIC CHEMISTRY – III (Paper 1)**  
**Sub Code: PG1731**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
6	5	90	100

### Objectives

- To acquire knowledge on principles involved in UV, NMR and Mass spectroscopy.
- To learn Woodward - Fischer rule and the calculation of  $\lambda_{\text{max}}$ .
- To study the McLafferty rearrangement and nitrogen rule.
- To gain knowledge about the synthesis, properties and structure of heterocyclic compounds.
- To learn the uses of the reagents in organic synthesis.

### Unit I: UV- Visible spectroscopy and IR spectroscopy

Basic principles of electronic transition. Absorption spectra of conjugated dienes,  $\alpha, \beta$  - unsaturated carbonyl compounds and aromatic compounds. Woodward - Fieser rule, Fieser - Khun rule, Scotts rule and Nielson rule. Effect of solvent polarity on  $\lambda_{\text{max}}$ . Applications.

IR: Principle, instrumentation and sampling techniques, Hooke's law, types of stretching and bending vibration. Factors influencing the vibrational frequency. Vibrational frequencies of alkane, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenol, amines, acids, esters and amides. Overtones and combination bands. Fermi resonance. FTIR (Principles only). Applications.

### Unit II: NMR Spectroscopy

$^1\text{H}$  NMR Spectroscopy: Instrumentation, principle of NMR spectroscopy, Chemical shift and substitution effects leading to empirical correlation for  $^1\text{H}$  chemical shifts and anisotropic shift. Spin-spin splitting. Types of coupling - germinal, vicinal, long range and through space coupling. Coupling constant - AB,  $\text{AB}_2$  and  $\text{A}_2\text{B}_3$ . Simplification of complex spectra - chemical exchange, double resonance and NMR shift reagents. FT-NMR.

<sup>13</sup>C NMR Spectroscopy: Principle, chemical shift, factors affecting chemical shift, broad band decoupling and OFF - resonance decoupling, coupling constants of aliphatic, aromatic and carbonyl carbons. 2D - NMR, COSY-HOMCOR, HETCOR and DEPT Technique, Comparison of <sup>13</sup>C NMR and <sup>1</sup>H NMR

### Unit III: Mass Spectroscopy

Basic principle, instrumentation production of ions, EI, CI, FAB – molecular ion peak, Base peak, meta stable peak and isotopic peaks. Nitrogen rule. McLafferty rearrangement. Retro Diels Alder reaction, fragmentation pattern of simple organic compounds - alkenes, halogens, alkyl benzene, benzene, aliphatic and aromatic alcohols, acids, ketones and aldehydes. Application of mass spectroscopy, determination of structure - related problems combining <sup>1</sup>H, <sup>13</sup>C NMR, IR, UV and Mass spectroscopy.

Circular birefringence (CB), Circular dichroism (CD), Cotton effect, ORD, Kronig-Kramers relation, applications of axial haloketone rule and octant rule.

### Unit IV: Heterocyclic Compounds

Synthesis, reactions and structure of indole, carbazole, oxazole, imidazole, thiazole, pyrones, coumarins, chromone. Structural elucidation of flavones, isoflavone and anthocyanins, caffeine, theobromine and theophylline.

### Unit V: Reagents in organic synthesis

Oxidation reactions involving SeO<sub>2</sub>, DDQ, DCC, 1,3-dithiane, NBS and m-CPBA, Aluminiumisopropoxide. Reduction involving complex metal hydrides - LiAlH<sub>4</sub>, NaBH<sub>4</sub>, DIBAL, Gilman's reagent, Tri-n-butyl tin hydride, 9-BBN, Wilkinson's catalyst, Vaska's catalyst and Baker yeast, Phase transfer catalysts, crown ether, LDA and Me<sub>3</sub>SiI, Fetizon's reagent, Lemieux-Von Rudloff reagent and Lemieux-Johnson reagent.

### Books for study

1. W. Kemp, Organic Spectroscopy, Macmillan, 3<sup>rd</sup>Edn., 1994.
2. Jag Mohan, Organic Spectroscopy Principles and applications, Narosa publishing house, 2001.
3. S.M. Silverstein, G.V. Bassler, T.C. Morrill, Spectrometric identification of organic compounds, Wiley, 6<sup>th</sup> Edn., 2004.
4. R.M. Acheson, Chemistry of Heterocyclic Compounds, Wiley Eastern Ltd., 1973.
5. V.K. Ahluwalia and R.K. Parashar, Organic reaction mechanisms, Narosa publishing house, 4<sup>th</sup> Edn., 2011.

### References.

1. J.R. Dyer, Applications of Absorption spectroscopy of Organic Compounds, Prentice Hall, 1987.
2. V.R. Dani, Organic spectroscopy, Tata McGraw Hill, 1995.
3. R.M. Acheson, An introduction to the chemistry of Heterocyclic compounds, Wiley Eastern Ltd., 2<sup>nd</sup> Edn., 1997.
4. K.S Tewari, N.K. Vishnoi, S.N. Mehrotra, A text book of organic chemistry, Vikas publishing House, Ltd. 2002.
5. T.W.G. Solomons, Organic Chemistry, Craig Fryhle Wiley, 2009.
6. M.T. Robert, R.N. Boyd, S.K. Bhattacharjee, Organic Chemistry, Pearson Education India, 7<sup>th</sup>Edn., 2011.

7. P.S. Kalsi, Organic Reactions and Mechanism, New Age International Ltd., 1<sup>st</sup> Edn., 1996.
8. G.R. Chatwal, Reaction Mechanism and Reagents in Organic Chemistry, Himalaya Publishing House, 5<sup>th</sup> Edn., 2016.

**SEMESTER – III**  
**PHYSICAL CHEMISTRY – III (Paper 3)**  
**Sub Code: PG1733**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
6	5	90	100

**Objectives**

- To know the various operations in Group Theory.
- To apply Group Theory to molecules.
- To understand the principle and applications of microwave and photoelectron spectroscopy.
- To understand the Chemistry of polymers.
- To know the role of radiations in Chemistry.

**Unit I: Group Theory - I**

Molecular symmetry elements and symmetry operations, molecular symmetry and point groups. Group multiplication tables - abelian, non - abelian, cyclic and sub groups - conjugacy relation and classes, representation of symmetry operations by matrices - representation of symmetry operations by matrices – representation for the  $C_{2v}$ ,  $C_{3v}$ ,  $C_{2h}$  to be worked out explicitly - reducible and irreducible representations, the great orthogonality theorem and its consequences without proof, construction of the character tables  $C_{2v}$ ,  $C_{3v}$ ,  $C_{4v}$ ,  $C_{2h}$  and  $D_{2d}$ .

**Unit II: Group Theory - II**

Standard reduction formula, Symmetry of normal modes of vibration in  $H_2O$ ,  $NH_3$ , and  $CO_2$ . Application of group theory to normal mode analysis ( $H_2O$ ,  $NH_3$ ). Symmetry properties of integrals and symmetry based selection rule for vibrational spectra -Identification of IR and Raman active fundamentals, symmetry of molecular orbitals and symmetry based selection rule for electronic transition, prediction of electronic transitions in ethylene and formaldehyde. Group theory applied to determine pi electron energy in ethylene - HMO theory - HMO calculations and delocalization energy in trans-1,3-butadiene and benzene. Group theory applied to determine hybridization scheme in  $CH_4$  and  $BF_3$ .

**Unit III: Molecular Spectroscopy - I**

Microwave spectroscopy: Rotation of molecules, Rotational spectra of diatomic molecules, intensity of spectral lines, effects of isotopic substitution, Non-rigid rotator. Rotational spectra of polyatomic molecules, chemical analysis by microwave spectroscopy. Photoelectron spectroscopy: Principle, photoelectric effect, Ionization process. Applications of photoelectron spectroscopy to simple molecules -  $O_2$  molecule,  $N_2$  molecule,  $CO$  molecule,  $NaN_3$ , Ethyl trifluoro acetate.

**Unit IV: Polymer Chemistry - I**

Homo and Hetero polymers, copolymer. Tacticity - Isotactic, atactic, syndiotactic Thermosetting and thermoplastics polymers. Linear, branched and cross linked polymers. Types of polymerisation - addition, condensation and co-polymerisation. Mechanism of addition

polymerisation - initiation, propagation and termination process. Initiators and inhibitors. Molecular mass - Number average, weight average, viscosity average molecular mass. Practical significance of molecular mass-distribution, size of polymers. Kinetics of polymerisation and Carather's equation.

### Unit V: Radiation Chemistry

Sources of high energy radiation, comparison of radiation chemistry with photochemistry, interaction of high energy radiation with matter. Experimental techniques - dosimetry and G-value, radiolysis of water, pulse radiolysis, hydrated electron, radiation chemistry in biology and industry (elementary aspects).

### Books for Study

1. P.K. Bhattacharya, Group Theory and its Chemical Applications, Himalaya Publishing house, 1986.
2. C.N. Ban Well, E.M. Mccash, Fundamentals of Molecular Spectroscopy, Tata Mc Grow Hill, New Delhi, 1997.
3. V.R. Gowariker, N.V. Viswanathan. J. Sreedhar, Polymer chemistry, New Age International Ltd, India, 1986.
4. S. Glasstone, Source Book on Atomic Energy, East West press, 3<sup>rd</sup> Edn., 1967.
5. H.J. Arikar, Elements of Nuclear Chemistry, Wiley Eastern Ltd., 4<sup>th</sup> Edn.,

### References

1. F.A. Cotton, Chemical Applications of Group Theory, Wiley, 3<sup>rd</sup> Edn., 2008.
2. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1998. K.V. Raman, Group Theory and its Applications to Chemistry, Tata Mcgraw Hill Publishing Co, 1990.
3. P. Ghosh, Polymer Science and Technology of Plastics and Rubbers, Tata McGraw – Hill Publishing Company, India, 1990.
4. P.W. Atkins, Physical Chemistry, Oxford University Press, 9<sup>th</sup> Edn., 2009.

**ELECTIVE PAPER**  
**ADVANCED TOPICS IN CHEMISTRY (Paper 4)**  
**Sub. Code: PG1734**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
4	4	90	100

### Objectives

- To acquire knowledge about nanoparticles and its growing technology.
- To learn the alternate methods of reaction by green chemistry.
- To gain an idea about supramolecular chemistry.
- To study the applications of medicinal and biophysical chemistry.

### Unit I: Nanochemistry

General principles of nanotechnology. Nanoparticles - definition, size relationship, nanoparticles of metals, semiconductors and oxides. Synthesis of nanosized compounds - Reduction methods, solgel method. Properties - optical and electrical properties. Nanosystems -

introduction, synthesis and purification of Fullerenes, Carbonnanotubes - preparation (Arc method, chemical vapour deposition method) and types. Gold and silver nanoshells and its applications. Nanosensors - introduction, nanoscale organization for sensors, characterization, nanosensors based on optical properties. Nanomedicines- introduction, approach to developing nanomedicines, protocol for nanodrug administration, diagnostic and therapeutic applications.

### **Unit II: Green Chemistry**

Definition, necessity for green chemistry. Green chemistry and sustainable development. Basic principles and applications of green chemistry. Atom economy – atom economy vs. yield in assessing greenness of organic reactions. Prevention of waste/byproducts. Prevention or minimization of hazardous products. Designing safer chemicals through Sommelet-Hauser, Cope, Wolff, Witting and Bamberger reactions. Energy requirement for synthesis. CFC alternatives – Example for green chemistry in organic synthesis. Selection of appropriate solvent and starting material. Use of protecting group and catalyst. Methods of greening organic reactions – solvent free reactions, reactions at ambient temperature. Microwave assisted reactions. Sonication assisted reactions – Reformatsky, Ullmann coupling, Wurtz and Bouveault reaction. Reactions in ionic solvents. Reactions in super critical fluids. Tandem reactions.

### **Unit III: Supramolecular Chemistry**

History, development and classification. Nature of supramolecular interactions - discussion of host-guest systems. Cation binding hosts-crown ethers, podates, cryptands, spherands. Anion binding hosts. Supramolecular chemistry of fullerenes. Molecular devices – non-linear optical switches, liquid crystal display. Supramolecular photochemistry.

### **Unit IV: Medicinal Chemistry**

Modern drugs for diseases - Antineoplastic agents: Classification, synthesis and assay of cyclophosphamide, and chlorambucil. Antimalarial drugs: Classification, synthesis and assay of chloroquine, and primaquine. Diuretics: Classification, synthesis and assay of Frusemide and benzthiazide. Anti-inflammatory drugs: Synthesis and therapeutic action of phenylbutazone, Ibuprofen. Antipyretics and Non-narcotic analgesics: Synthesis and therapeutic action of paracetamol, Aspirin

### **Unit V: Biophysical Chemistry**

Thermodynamics in biology - limitations of equilibrium thermodynamics. Irreversible thermodynamics - Postulates and methodologies. Onsager reciprocal theory. Irreversible thermodynamics and biological systems. Energy flux - biochemical standard state - ATP. Currency of energy - Oxidative phosphorylation. Role of Singlet Oxygen in biology. Reactions in biomolecules - membrane potential, ion pumps. Photoacoustic effect and its application in biology. Biophysical applications of Mossbauer effect. NMR imaging - Applications of spin labeling in membrane research.

### **Books for Study**

1. K.J. Klabunde, R.M. Richards, Nanoscale Materials in Chemistry, Wiley, 2<sup>nd</sup> Edn., 2009.
2. V. K. Ahluwalia, Strategies for Green Organic Synthesis, Taylor and Francis group, CRC Press, 2012.
3. A. Kar, Medicinal Chemistry, New Age International Publishers, 4th Edn., 2007.

### **References**

1. G. Ozin, A. Arsenault, Nanochemistry: A Chemical Approach to Nanomaterials, Elsevier, 2005.
2. C.N.R. Rao, Nanochemistry, Wiley Inter Science, New York, 2001.

3. H. Nalwa, Nanostructured Materials and Nanotechnology, Academic Press, 1998.
4. A. Matlack, Introduction to Green Chemistry, Taylor and Francis group, CRC Press, 2nd Edn., 2010.
5. K. Ilango and P. Valentina, Text Book of Medicinal chemistry, Keerthi Publishers, 4<sup>th</sup>Edn., 2009

**SEMESTER – III**  
**ELECTIVE PAPER**  
**PHARMACEUTICAL CHEMISTRY (Paper 4)**  
**Sub Code: PG1734**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
4	4	90	100

**Objectives**

- To gain knowledge on mechanism of drugs action and its function
- To learn the chemicals involved in the cure of different diseases
- To study about blood grouping and related tests
- To acquire knowledge on Indian medicinal plants

**Unit I**

Important terminologies - Molecular Pharmacology, pharmacophore, Metabolites, Antimetabolites, virus, bacteria, fungi, actinomycetes, mutation - Classification of drugs - Nomenclature of drugs - non proprietary names – source, assay (biological, chemical, immunological) - Testing of potential of drugs and their side effects.

**Unit II**

Mechanism of drug action - absorption, drug delivery, drug excretion - physiological effects of different functional groups in drugs - Indian Medicinal plants and trees (Tulsi, Neem, Keezhanelli, Adathode, Thoothuvalai) Biological role of salts of Na, K, and Ca, Cu, Zn and Iodine. (Source and deficiency) Uses of the following: MgSO<sub>4</sub>, 7H<sub>2</sub>O, Milk of Magnesia, Magnesium Trisilicate, Aluminium Hydroxide gel, - HgCl<sub>2</sub>, HgI<sub>2</sub>, and Hg (CN)<sub>2</sub> as disinfectant.

**Unit III**

Analgesics - Salicylates - Narcotics, Opiates - Morphine, Pethidine, Anaesthetics - Local anaesthetics - Procaine and related compounds - General anaesthetics - Chloroform ether and barbiturates - Antipyretics - paracetamol and other p-aminophenol derivatives - antiseptics and disinfectants - distinction - phenols, chloramines, cyclohexadiene, organomercurals - Antibiotics. Therapeutic values of penicillin, streptomycin, chlormphenicol and tetracyclines - Hypoglycemic drugs - insulin - oral hypoglycaemic agents - sulphonylureas, Hypnotics, tranquilizers and sedatives - Drugs addiction.

**Unit IV**

Common diseases - causes and treatment - insect borne diseases (Malaria, Filariasis) - Airborne disease (Diphtheria, Whooping cough, Influenza, TB) - Waterborne diseases (cholera, typhoid, dysentery) - Jaundice and Leprosy - First aid for accidents - cuts, bleeding, fractures, burns, fainting, poisonous bites and poisoning.

## Unit V

Blood grouping - Rh factor - Tests for Urea and Cholesterol - Role of blood as Oxygen carrier - Clotting mechanism - Blood pressure - Causes and control - Causes of anaemia - Antianaemic drugs, cardiovascular drugs, cardiglycosides, antianginal agents, vascodilators, (one example for each).

Causes for cancer, antineoplastic agents - Cobalt therapy - AIDS - Causes, HIV virus, propagation, prevention and treatment.

### Reference:

1. A. Kar, Medicinal Chemistry, Medicinal Chemistry, New Age international Ltd., 4thEdn., 2006.
2. D. Cairns, Essentials of Pharmaceutical Chemistry, Pharmaceutical Press, 4<sup>th</sup> Edn., 2012.
3. J. Barber, C. Rostron, Pharmaceutical Chemistry, Oxford University Press, 1<sup>st</sup> Edn., 2013.
4. J. Ghosh, A Textbook of Pharmaceutical Chemistry, S. Chand & Company Ltd, 2014
5. G.R. Chatwal, M. Arora, Pharmaceutical Chemistry-Inorganic (Vol. I), Himalaya Publication. House, 2010.
6. G.R. Chatwal, M. Arora, Pharmaceutical Chemistry Organic (Vol. II), Himalaya Publication. House, 2008.

## NORGANIC CHEMISTRY PRACTICAL - II

(III and IV Semester)

Sub Code: PG17P4

### Objectives

- To carry out the titrimetric and gravimetric analyses.
- To perform the preparation of compounds.

1. Separation and estimation of metal ions in a mixture by volumetric and gravimetric methods. Some typical recommended mixtures are:

Cu(II) and Ni(II)  
Fe(II) and Cu(II)  
Cu(II) and Zn(II)  
Ca(II) and Ba(II)  
Fe(II) and Ni(II)

2. Preparation of complexes:

Tris(thiourea)copper(I) chloride  
Tetraamminecopper(II) sulphate  
Potassium trioxalatoferrate  
Potassium trioxalatoaluminate(III)  
Potassium trioxalatochromate(III)  
Hexamminecobalt(III) chloride



## References

1. A.I. Vogel, Text Book of Quantitative Inorganic Analysis; 6th Ed., Longman, New Delhi, 2000.
2. V.V. Ramanujam, Inorganic Semimicro Qualitative analysis, The National publishing Co., Chennai, 3<sup>rd</sup> Edn., 1988.

**SEMESTER – IV**  
**ORGANIC CHEMISTRY – IV (Paper 1)**  
**Sub Code: PG1741**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
6	4	75	100

## Objectives

- To impart idea about retrosynthetic analysis.
- To study the nature of alkaloids, extraction, and its general properties.
- To gain knowledge on molecular rearrangements.
- To learn photochemical reactions, Norrish type-I and type-II reactions.
- To enable the students with the knowledge of pericyclic reactions.

### Unit I: Retrosynthetic Analysis

Planning – relay, linear and convergent approach, protecting groups and activating groups. Target molecule containing one functional group requiring a single disconnection - synthons and synthetic equivalents. Latent polarity. Target molecules with two functional groups - 1,3-, 1,5- and 1,4-dicarbonyl compounds. Functional group interconversions. Umploung synthesis. Retrosynthetic analysis of bisabolene, cis-Jasmone and longifolene. Stereo selective problems of geometrical and optical isomerism-diastereo selectivity and enantioselectivity.

### Unit II: Alkaloids

Alkaloids, Extraction, general properties, classification, general methods for determining structure. Structural elucidation –morphine, atropine, cocaine, tropaine, quinine, papaverine.

### Unit III: Molecular rearrangements

Classification – electrophilic, nucleophilic and free radical rearrangements. Mechanisms of the following rearrangements – Wagner Meerwin, Tiffenev- Demyanov, Dienone- Phenol, Favorskii, Fries, Baeyer – Villager, Stevens, Neber, Sommelet-Hauser, Baker-Venkatraman, von-Richter rearrangement and Di-  $\pi$ - methane rearrangement.

### Unit IV: Organic Photochemistry

General introduction. Thermal versus photochemical reactions, Jablonski diagram. Photochemical reactions of ketones – Photosensitization, Norrish type - I and Norrish type - II reactions and mechanisms, Paterno - Buchireaction,Photooxidationandphotoreduction of ketones , Photochemistry of arenes.

Photodimerisation, photoisomerisation.Reactions involving free radicals-Barton reaction, Hunsdiecker reaction.Pschorr reaction and Gomberg-Bauchman reaction.

### Unit V: Pericyclic Reactions

Characteristics and classifications of pericyclic reactions - electrocyclic, cycloaddition and sigmatropic reactions.

- a) Woodward Hofmann rule
- b) 2+2, 2+4 - reactions

- c) Retro-Diels Alder reaction
- d) Diels Alder reaction
- e) Cope rearrangements
- f) Claisen rearrangements

Conservation of orbital symmetry – Prediction of reaction conditions using FMO, correlation diagrams and Zimmerman (Möbius - Hückel analysis) approaches.

### Books for Study

1. K. S. Tewari, N. K. Vishnoi, S.N. Mehrotra, A Text Book of Organic Chemistry, Vikas publishing House Ltd. 2002.
2. O.P. Agarwal, Chemistry of Organic Natural Product, Vol. I and Vol. II, Goel Publishing House, 1947.
3. V.K. Ahluwalia, R.K. Parashar, Organic Reaction Mechanisms, Narosa publishing house, 4<sup>th</sup> Edn., 2011.
4. C.H. Depuy, O.S. Chapman, Molecular Reactions and Photochemistry, Prentice Hall of India Private Limited, July 1988.
5. G.B. Gill, M.R. Wills Pericyclic Reactions, Chapman and Hall, London 1974.

### References

1. M.K. Jain, S.C. Sharma, Modern Principles of Organic Chemistry, Vishal publication, 2014.
2. J. March, Advanced Organic Chemistry, Wiley, 4<sup>th</sup> Edn., 2003.
3. R. T. Morrison, R. N. Boyd, Organic Chemistry, Prentice Hall, 6<sup>th</sup> Edn., 1997.
4. I.L. Finar, Organic Chemistry, Vol. I and II, ELBS, 5<sup>th</sup> Edn., 2001.
5. O. P. Agarwal, The Chemistry of Organic Natural Product Vol. I and Vol. II, Geol publishing House 1947.

**SEMESTER – IV**  
**INORGANIC CHEMISTRY – IV (Paper 2)**  
**Sub Code: PG1742**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
5	4	75	100

### Objectives

- To gain knowledge about various spectroscopic techniques in inorganic chemistry.
- To understand the principles of nuclear reactions.
- To acquire knowledge in different properties of solids.
- To know the concepts of bio-inorganic chemistry.

### Unit I: Application of spectroscopy to the study of inorganic compounds - III

NMR Spectroscopy: Principle, <sup>31</sup>P, <sup>19</sup>F, <sup>15</sup>N, applications in structural problems. Monitoring the course of reaction. NMR of fluxional molecules. NMR of paramagnetic molecules - contact shift and shift reagents.

NQR Spectroscopy: Principle, comparison with NMR, electric field gradient, quadrupolar splitting of energy levels in symmetric and asymmetric fields, quadrupolar coupling in atoms and

molecules, asymmetry parameter. Application - hydrogen bonding, phase transition, substituent effect and structural information.

#### **Unit II: Applications of spectroscopy to the study of inorganic compounds - IV**

ESR spectroscopy: Principles, presentation of the spectrum, hyperfine splitting, factors affecting the magnitude of g values, zero-field splitting and Kramer's degeneracy, anisotropy in the hyperfine coupling constant. Covalency of M-L bonding by ESR. Jahn- Teller distortion in Cu (II) complexes from ESR studies.

Mossbauer Spectroscopy: Principle, Doppler Effect, recoil energy, minimizing recoil energy, Doppler broadening. Isomer shift - isomer shift in Fe and Sn compounds. Electro negativity and chemical shift. Quadrupole interaction - quadrupole splitting in the MB spectra of Fe complexes. Applications of MB spectroscopy.

#### **Unit III: Nuclear Chemistry**

Thermal and nuclear reactions, Q-value, Capture cross section, threshold energy and excitation functions. Nuclear models-Shell model, Liquid drop model, Fermi gas model, Collectur model, optical model. Types of nuclear reactions - Nuclear fission, characteristics, product distribution, theories of fission. Nuclear fusion and stellar energy. Nuclear materials and waste disposal.

#### **Unit IV: Electrical and magnetic properties of solids**

Conductivity of pure metals - Electrical conductivity, photoconductivity, photoconductive device. Solar cell, solar energy conversion. Dielectric properties - permittivity, dielectric constant, electric susceptibility, electronic polarization, ionic polarization, orientation, dielectric loss and dielectric break down, Ferro electricity. Applications of magnetic properties of solids - dia, para, ferro, antiferro and ferri magnetism. Effect of temperature on magnetism - Curie and Weiss law. Calculation of magnetic moments.

#### **Unit V: Bio Inorganic Chemistry - II**

Photosynthesis, photosystem I and II, photosynthetic reaction center. Metallo enzymes: Enzymes in di-oxygen management – Super oxide dismutase, superoxide toxicity, structure of Cu, Zn-SOD, Enzymatic activity and mechanism. Peroxidases and catalases, oxidases and mono oxygeneases, Zinc enzymes – the structural role of Zinc and Zinc constellations of carbonic anhydrase, carboxy peptidase and alcohol dehydrogenase. Metal complexes as probes of nucleic acids. Gold compounds and anti-arthritis agents.

#### **Books for Study**

1. E. Horwood, NMR, NQR, EPR, and Mössbauer Spectroscopy in Inorganic Chemistry, 2010.
2. H.J. Arnikaar, Essentials of Nuclear Chemistry, Wiley Eastern Ltd., 4<sup>th</sup> Edn., 2000.
3. L.V. Azaroff, Introduction to Solids, Tata McGraw Hill Publishing Ltd., India, 1989.
4. G.R. Chatwal, A.K. Bhagi, Bio-inorganic Chemistry, Himalaya Publishing House, 2<sup>nd</sup> Edn., 2005.
5. A.K. Das, Bio-inorganic Chemistry, Books and Allied (P) Ltd., 2007.

#### **References**

1. A.K. Brisdon, Inorganic Spectroscopic Methods, OUP Oxford, 1998.
2. J.A. Iggo, NMR Spectroscopy in Inorganic Chemistry, OUP Oxford, 2000.
3. R.K. Puri, V.K. Babber, Solid State Physics, S. Chand and Company Ltd., 2001.
4. A.R. West, Solid State Chemistry and Applications, Jhon-Wiley and Sons, 1987.

- Gary L. Miessler, Inorganic Chemistry, Pearson Education Inc., 3<sup>rd</sup> Edn., 2004.
- S. Glasstone, Source Book of Atomic Energy, East West Pvt. Ltd., 1969.
- G. Friedlander, J.W. Kennedy, N.M. Miller, Nuclear and Radio Chemistry, John Wiley, 1981.
- J.E. Huheey, E. A. Keiter, R.L. Keiter, O.K. Medhi, Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education, 4<sup>th</sup> Edn., 2011.
- W.U. Malik, G.D. Tuli, R.D. Madan, Selected topics Inorganic Chemistry, S. Chand Company Ltd., 2012.

**SEMESTER – IV**  
**PHYSICAL CHEMISTRY – IV (Paper 3)**

**Sub Code: PG1743**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
5	4	75	100

**Objectives**

- To gain knowledge about polymers.
- To know the importance of various spectroscopic techniques.
- To study the structures of various crystals.

**Unit I: Polymer chemistry - II**

Conducting Polymers. Factors affecting the conductivity of conducting polymers. Doping of conducting polymers. Degradation of polymers, types of degradation - thermal degradation, mechanical degradation, oxidative degradation, degradation by ultrasonic waves, degradation by high energy radiation and photodegradation. Glass transition temperature, crystallinity in polymers. Viscosity, solubility, optical, electrical, thermal, and mechanical properties of polymers. Polymers processing - compression moulding, injection moulding, transfer moulding and extrusion moulding. Casting extrusion of fibres, spinning.

**Unit II: Polymer chemistry - III**

Synthesis of intermediates - Terephthalic acid, DMT, caprolactam, hexamethylenediamine, ethylene glycol, adipic acid, acrylonitrile. Synthetic polymers - synthesis, properties and applications of polyethylene - HDPE, LDPE, LLDPE - polypropylene - polyvinyl chloride - grades of PVC - Teflon, polymethylmethacrylate (plexiglass) polystyrene - Homopolymers, copolymers (SBR, ABS, SAN) polyester, polyamide – Nylon-66. Natural polymers – Cellulose, starch, silk, wool - Cellulose acetate, cellulose nitrate. Polymers in medicine and surgery. Biomedical applications of polymers.

**Unit III: Molecular Spectroscopy - II**

Electronic Spectroscopy: Principle, laws of light absorption, Born-Oppenheimer approximation. Franck-Condon principle, Wave-mechanical formulation, dissociation energy and dissociation products, predissociation, fluorescence & phosphorescence - principle and theory.

Nuclear magnetic resonance spectroscopy: Principle, Nuclear spin and nuclear moment, chemical shift and its measurements, factors influencing chemical shift, shielding and deshielding effects, spin-spin interactions, NMR of simple AMX type molecules, coupling constant, FTNMR, NMR of <sup>19</sup>F, <sup>31</sup>P and <sup>13</sup>C .

#### Unit IV: Molecular Spectroscopy - III

ESR: Theory, hyperfine interactions in ESR. Double resonance (ENDOR, ELDOR), McConnell's relation - verification of the relation for cyclic polyene radical and calculation of electron density. Experimental Techniques.

Laser Raman Spectroscopy: Einstein treatment of absorption and emission phenomena. Einstein's coefficients. Probability of induced emission and its applications to lasers. Conditions for laser action. Properties and types of lasers. Advantages of lasers in Raman spectroscopy. Experimental Techniques.

#### Unit V: Solid State Chemistry

Space lattices, X-ray diffraction, Bragg's equation, rotating crystal method and powder method, ionic radii and Gold Schmit's rule, closed packing in solids - structure of typical lattices Perovskite, CsCl, Zinc blende, Wurtzite, Rutile, fluorite, Antifluorite, covalent crystals - diamond and graphite.

#### Books for Study

1. V.R. Gowariker, N.V. Viswanathan. J. Sreedhar, Polymer chemistry, New Age International Ltd, India, 1986.
2. C.N. Ban Well, E.M. Mccash, Fundamentals of Molecular Spectroscopy, Tata Mc Grow Hill, New Delhi, 1997.
3. L.V. Azaroff, Introduction to Solids, Tata McGraw Hill Publishing Ltd., India, 1989.

#### References

1. P. Ghosh, Polymer Science and Technology of Plastics and Rubbers, Tata McGraw – Hill Publishing Company, India, 1990.
2. Fred W. Billmeyer, Textbook of Polymer science, Wiley Interscience publication, New York, 1984.
3. R. Chang, Basic principles of spectroscopy, Tata McGraw Hill, 1971.
4. G. Aruldas, Molecular Structure and Spectroscopy, PHI Learning Pvt. Ltd, 2<sup>nd</sup> Edn., 2011.
5. C. Kittel, Introduction to Solid State Physics, Tata McGraw Hill 7<sup>th</sup> Edn., 1996.

### SEMESTER – IV Energy for the Future

Sub Code: PG1744

Elective / Non-Major Elective

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
5	4	75	100

#### Objectives

- To acquire knowledge on conventional and non-conventional energy sources.
- To enlighten the students with knowledge of solar radiation and its measurement.
- To study the principles and applications of wind energy.
- To learn the properties and utilization of biogas.
- To know about fuel cells and hydrogen energy.

## **Unit I Introduction to Energy Sources**

Introduction, conventional energy sources like coal, oil, gas, agricultural and organic wastes, water power, thermal power and nuclear power. Non-conventional energy sources like solar energy, wind energy, energy from bio-mass and bio-gas, ocean thermal energy, tidal energy, geothermal energy and hydrogen energy. Advantages of renewable energy.

## **Unit II Solar Energy**

Solar radiation and its measurement: Introduction, solar constant, solar radiation at the earth's surface, solar radiation geometry and solar radiation data. Solar energy collectors: Introduction, physical principles of the conversion of solar radiation into heat, flat plate and concentration collectors. Advantages and disadvantages of concentration collectors over flat collectors. Energy balance equation and collector efficiency.

## **Unit III Wind Energy**

Introduction, basic principles of wind energy conversion, power of the wing, forces on the blades. Wind energy conversion, wind data and estimation, site selection. Types of wind machines – Horizontal axis machine – vertical axis machine. Analysis of aerodynamic forces acting on the blade, performance of wind machines. Generating systems: Introduction, schemes of electric generation, generator control, load control, energy storage. Application of wind energy.

## **Unit IV Bio-energy**

Introduction, biomass conversion techniques – wet processes and dry processes. Biogas generation. Classification of biogas plants: floating drum plant and fixed dome type plant. Biogas from plant waste. Materials used for biogas generation, selection of site for a biogas plant, digester design. Problems related with biogas plants. Fuel properties of biogas and utilization of biogas.

## **Unit V Chemical energy sources**

Fuel cells: Introduction, conversion efficiency of fuel cells, types of electrodes, work output and EMF of fuel cells, applications of fuel cells. Hydrogen energy: Hydrogen production – electrolysis – thermo-chemical methods, fossil fuel methods and solar energy methods. Hydrogen storage and hydrogen transportation. Utilization of hydrogen gas – hydrogen as an alternative fuel for motor vehicles. Safety and management.

## **References**

1. G.D. Rai, Non-conventional Energy Sources, Khanna Publications, 2004.
2. R. Wengenmayr, T. Bührke, W.D. Brewer, Renewable Energy: Sustainable Energy Concepts for the Energy Change, Wiley VCH, 2<sup>nd</sup> Edn., 2012.
3. V. Nelson, Introduction to Renewable Energy (Energy and the Environment), CRC Press, 2011.
4. J. Twidell, T. Weir, Renewable Energy Resources, Taylor and Francis, 2<sup>nd</sup> Edn., 2006.
5. D. Chiras, Achieving Energy Independence through Solar, Wind, Biomass and Hydropower, Mother Earth News Wiser Living, 2006.
6. J.W. Tester, E.M. Drake et al., Sustainable Energy, Prentice-Hall of India, New Delhi, 2006.

**Semester IV**  
**Nanochemistry (Elective IV)**  
**Sub. Code: PG1745**

Number of Hours Per week	Number of Credit	Total No. of hours	Marks
6	5	90	100

**Objectives:**

1. To acquire knowledge about basic concepts of nanochemistry.
2. To study the synthesis of nanomaterials.
3. To gain knowledge on the characterization techniques of nanomaterials.
4. To understand the applications of carbon clusters.
5. To learn about nanodevices and its applications.

**Unit I: Basic concepts of nanochemistry**

Introduction to nanoscience and nanotechnology, discussion on various phenomenon at nanoscale, such as size, shape, surface, surface energy, surface stabilization, characteristic length, self-assembly, defects, size quantization, surface plasmon, conductivity, tunneling, magnetism, defects.

**Unit II: Synthesis of nanomaterials**

Basics of nanofabrication method - top-down, bottom-up approaches, gas phase, liquid phase, solid phase synthesis, self-assembly, templated synthesis, sol-gel, electrodeposition, fundamentals of nanoparticle formation, thermodynamic approach, supersaturation, nucleation, growth, homo vs hetero nucleation. Synthesis of nanoparticles: metallic, semiconducting, quantum dots, oxides, hybrids, micelles and microemulsion as templates for synthesis. 0D, 1D and 2D nanoparticles, core-shell nanoparticles, special nanoparticles, shaped nanoparticles.

**Unit III: Characterization techniques**

Discussion on various techniques available for characterizing the nanomaterials for their size, shape, morphology, crystalline phase, oxidation states, textural properties (surface area, pore volume, pore size), thermal stability, light absorption and band gap. Scanning electron microscope (SEM), Transmission electron microscope (TEM), X-ray powder diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Scanning tunnelling microscope (STM) and Atomic force microscope (AFM). Thermal analysis, N<sub>2</sub> sorption techniques for textural properties of the material solid state NMR for characterizing functionalized materials.

**Unit IV: Carbon clusters and nanostructures**

Bonding in carbon, new carbon structures, carbon clusters, discovery of C<sub>60</sub>, alkali doped C<sub>60</sub>, superconductivity in C<sub>60</sub>, larger and smaller fullerenes. Carbon nanotubes - synthesis, single walled carbon nanotubes, structure and characterization, mechanism of formation, chemically modified carbon nanotubes, doping, functionalizing nanotubes, application of carbon nanotubes, nanowires, synthetic strategies, gas phase and solution phase growth, growth control, properties.

**Unit V: Nanotechnology and Nanodevices**

DNA as a nanomaterial. DNA - knots and junctions. DNA nanomechanical device designed by Seeman. Force measurements in simple protein molecules and polymerase. DNA complexes. Molecular recognition and DNA based sensor. Protein nanoarray, nanopipettes, molecular diodes, self-assembled nanotransistors and nanoparticle mediated transfection.

### Text Books

1. Rao, C.N.R., Muller, A. & Cheetam, A.K. (2004). The Chemistry of Nanomaterials. Vol. I. New York: Wiley-VCH.
2. Poole, C.P. & Owens, F.J. (2003). Introduction to Nanotechnology. New Jersey: Wiley Interscience
3. Klabunde, K.J. (2001). Nanoscale materials in Chemistry. New York: Wiley-Interscience.
4. Pradeep, T. (2007). Nano: The Essentials in Understanding Nanoscience and Nanotechnology. New Delhi: Tata McGraw Hill.

### Reference Books

1. Rao, C.N.R., Muller, A. & Cheetam, A.K. (2004). The Chemistry of Nanomaterials. Vol.I. New York: Wiley-VCH.
2. Tang, T. & Sheng, P. (2004). Nano Science and Technology-Novel Structures and Phenomena. New York: Taylor and Francis.
3. Heiz, U. & Landman, U. (2006). Nanocatalysis. New York: Springer.

## PHYSICAL CHEMISTRY PRACTICAL - I (III and IV Semester) Sub Code: PG17P3

### Potentiometry

1. Determination of solubility product of sparingly soluble salts using AgCl.
2. Determination of dissociation constant of a weak acid.
3. Potentiometric titrations.
  - a) Redox titrations
    - (i)  $\text{Fe}^{2+}$  vs  $\text{Cr}_2\text{O}_7^{2-}$
    - (ii)  $\text{I}^-$  vs  $\text{MnO}_4^-$
    - (iii)  $\text{Fe}^{2+}$  vs  $\text{Ce}^{4+}$
  - b) Precipitation titrations
    - (i)  $\text{Cl}^-$  vs  $\text{AgNO}_3$
    - (ii)  $\text{I}^-$  vs  $\text{AgNO}_3$
    - (iii) Mixture of  $\text{Cl}^-$  and  $\text{I}^-$  vs  $\text{AgNO}_3$
4. Determination of strength of oxalic acid from the study of its adsorption on activated charcoal.
5. Conductivity:
  - a) Estimation of the strength of strong acid.
  - b) Estimation of the strength of weak acid.
  - c) Estimation of the strength of  $\text{NH}_4\text{Cl}$ .
  - d) Estimation of the strength of HCl and  $\text{NH}_4\text{Cl}$  in a mixture.
  - e) Estimation of the strength of strong and weak acids in a mixture
6. Estimation of Thermometric Experiments:  
Determination of heat of solution-  
Ammonium oxalate and water  
Naphthalene and toluene



## References

1. B. Viswanathan, P.S Raghavan, Practical Physical Chemistry, Viva Books Ltd., 2005.
2. M.J. Sienko, R.A. Plane, S.T. Martu, Experimental Chemistry, International student Edn.,1984.
3. D.P. Shoemaker, C.W. Garland, J.W. Nibler, Experiments in Physical Chemistry, McGraw Hill International Edn., 1974.
4. B.P. Levitt, Findlay's Practical Physical Chemistry, 9<sup>th</sup> Edn., 1972.  
A.M. James, F.E. Prichard, Physical Chemistry Practicals, 3<sup>rd</sup> Edn.,