

**M. Sc CHEMISTRY – COURSE PATTERN – 2016 SET**

Sem.	Code	Course Title	Hrs/Wk	Credits
I	16PCH1101	Inorganic Chemistry I	6	5
	16PCH1102	Organic Chemistry I	6	5
	16PCH1103	Physical chemistry I	6	5
	16PCH1104	Organic Chemistry Practical I	4	3
	16PCH1105	Physical Chemistry Practical I	4	3
	16PPH1401	IDC-1(W.S) Physics for Competitive Examinations	4	4
	<i>Total for Semester I</i>			<b>30</b>
II	16PCH2106	Inorganic Chemistry II	6	5
	16PCH2107	Organic Chemistry II	6	5
	16PCH2108	Physical chemistry-II	6	5
	16PCH2109	Organic Chemistry Practical II	4	3
	16PCH2110	Physical Chemistry practical-II	4	3
	16PCH2111	Self-Paced Learning: Natural Products	-	2
	16PSS2401	IDC: Soft Skills	4	4
<i>Total for Semester II</i>			<b>30</b>	<b>27</b>
III	16PCH3112	Inorganic Chemistry III	6	5
	16PCH3113	Organic Chemistry III	6	5
	16PPS3101	Common Core: Methods of Spectroscopy and Lasers	6	5
	16PCH3114	Inorganic Chemistry Practical I	4	3
	16PCH3202A	Elective II A: Thermodynamics I OR	4	4
	16PCH3202B	B: Thermodynamics II		
	16PCH3402	IDC: (BS) Health Chemistry	4	4
<i>Total for Semester III</i>			<b>30</b>	<b>26</b>
IV	16PCH4115	Inorganic Chemistry IV	4	4
	16PCH4116	Organic Chemistry IV	4	4
	16PCH4117	Inorganic Chemistry Practical II	4	4
	16PCH4118	Comprehensive Examination	-	2
	16PCH4202A	Elective: Physical Chemistry III OR	4	4
	16PCH4202B	Polymer Chemistry		
	16PCH4203A	Elective: Analytical Chemistry OR	4	4
	16PCH4203B	Pharmaceutical Chemistry		
	16PCH4501	Project Dissertation & Viva Voce	10	5
<i>Total for Semester IV</i>			<b>30</b>	<b>27</b>
I- IV	SHEPHERD & Gender Studies		-	5
<i>Total For All Semesters</i>			<b>120</b>	<b>110</b>

Sem. I  
16PCH1101

Hours/Week: 6  
Credits: 5

## INORGANIC CHEMISTRY-I

### *Assurance of Learning*

- Chemistry of transition and inner transition elements are learnt
- Fundamentals and instrumentation of nuclear chemistry are learnt
- Applications of nuclear chemistry and radioactivity are learnt

### Unit I

#### Transition Elements

(16 Hours)

Transition elements – General characteristics – atomic, ionic radii – variation along the period and group – variable valency, colour, magnetic properties, non-stoichiometry, catalytic property and complexing tendency – Stabilization of unusual oxidation states.

### Unit II

#### Inner Transition Elements

(16 Hours)

Inner transition elements – position in the periodic table – electronic configuration, oxidation states, solubility, colour and spectra, magnetic properties – Separation of lanthanides – lanthanide contraction: Cause and consequences – Gadolinium break, shift reagents – Extraction of thorium and uranium. Comparison of actinides and lanthanides

### Unit III

#### Selected Compounds of d-block elements and fundamentals of nuclear chemistry

(16 Hours)

Selected Compounds of *d*-block elements (Structure only): Chromium(II) acetate, Manganese(III) acetate, Manganese(III) oxalate,  $[\text{Re}_2\text{Cl}_8]^{2-}$ ,  $[\text{Nb}_6\text{Cl}_{12}]^{2+}$ ,  $[\text{Mo}_6\text{Br}_8]^{4+}$ ,  $[\text{Ni}(\text{dmg})_2]$ ,  $[\text{Zn}(\text{edta})]$ , basic zinc acetate

#### Fundamentals of Nuclear Chemistry

(16 Hours)

The nucleus – subatomic particles and their properties - nuclear binding energy – nuclear structure – Liquid drop model and nuclear shell model – *n/p* ratio - nuclear forces - Modes of radioactive decay – alpha, beta and gamma decay – orbital electron capture – nuclear isomerism – internal conversion

### Unit IV

#### *ON-LINE*

#### Instrumental Techniques in Nuclear Chemistry

(16 Hours)

Q value of nuclear reaction, Coloumbic barrier, nuclear cross section, threshold energy and excitation function – Different types of nuclear reactions fragmentation, nuclear fission, nuclear fusion – proportional counter, Geiger-Muller counter, scintillation counter and Cherankov counter. Linear accelerators – cyclotron, synchrotron

### Unit V

#### Applications of Fission, Fusion and Trace Elements

(16 Hours)

Characteristics of fission reactions – product distribution of fission, theories of fission – fissile and fertile isotopes – nuclear fusion and stellar energy, synthetic elements – Nuclear wastes – nuclear reprocessing – radiation hazards and prevention. Applications of isotopes – neutron activation analysis – isotopic dilution analysis – Uses of tracers in structural and mechanistic studies, agriculture, medicine and industry – Radio carbon dating - hot atom chemistry – Atomic Power Projects in India.

## TEXTBOOKS

1. Lee J D, *Concise Inorganic Chemistry*, 6e, ELBS, London, 1998
2. Huheey J E, Keiter E A and Keiter R L, *Inorganic Chemistry Principles of Structure and Reactivity*, 4e, Harper Collins College Publishers, New York, 1993
3. Glasstone S, *Sourcebook on Atomic Energy*, Affiliated East West Press Pvt. Ltd., New Delhi, 1967

## REFERENCES

1. Cotton F A and Wilkinson G, *Inorganic Chemistry A Comprehensive Text*, 3e, Interscience Publishers, New York, 1972
2. Purcell K F and Kotz J C, *Inorganic Chemistry*, W B Saunders Company, Philadelphia, 1977
3. Shriver D, Weller M, Overton T, Rourke J and Armstrong F, *Inorganic Chemistry* 6e, W H Freeman and Company, New York, 2014
4. Miessler G L, Fischer P J and Tarr D A, *Inorganic Chemistry*, 5e, Pearson Education, Inc., New York, 2014
5. Housecroft C E and Sharpe A G, *Inorganic Chemistry* 4e, Pearson Education Limited, Essex, 2012
6. Friedlander G, Macias E S, Kennedy J W and Miller J M, *Nuclear and Radiochemistry*, 3e, John Wiley and Sons Inc., London, 1981
7. Arniker H J, *Essentials of Nuclear Chemistry*, New Age International Publishers, New Delhi, 2005
8. Choppin G, Liljenzin J, Rydberg J and Ekberg C, *Radiochemistry and Nuclear Chemistry*, 4e, Elsevier, Amsterdam, 2013

<b>Sem: I</b>		<b>Hours: 6</b>
<b>Code: 16PCH1102</b>	<b>ORGANIC CHEMISTRY I</b>	<b>Credits: 5</b>

### Learning Assurances

After learning these topics the students have sufficient knowledge on the following:

1. The concept of bonding and structure
2. The stereochemistry of organic molecules
3. The kinetic and mechanistic aspects of organic reactions

### Unit I: Bonding, Structure & Aromaticity

**Hybridization** with reference to carbon compounds-Shapes of simple organic molecules-bond angle and bond length in organic molecules. Electronegativity of atoms and groups. Dipole moments of molecules-Applications of dipole moment to study the properties of organic molecules. Polarity of solvents. Hydrogen bonding-Inter and Intramolecular hydrogen bonding. **Electronic Effects**-Inductive, resonance and hyperconjugative effects and their influence-rules of resonance. Tautomerism. Steric effects.

**Aromaticity:** Aromatic character-Huckel's rule and applications-Craig's rule and applications-Consequences of aromaticity - non-alternation in bond length-Resonance energy from heat of hydrogenation, heat of combustion and Huckel's MO calculation, antiaromatic compounds-paratropic compounds.

### Unit II: Essentials of Organic Stereochemistry

Principles of symmetry-concept of chirality. Molecular symmetry and chirality. Newmann, Sawhorse, Fischer and Wedge representations and their interconversions. Types of molecules exhibiting optical activity. Configurational nomenclatures of acyclic and cyclic molecules: *cis-trans* and *E,Z* - and *D, L; R, S; erythro* and *threo; syn* and *anti; endo* and *exo*.

Stereochemistry of molecules with axial chirality-atropisomerism - biphenyls-allenes, spiranes and analogues. Helicity and chirality. Topocity and prostereoisomerism-topocity of ligands and faces-enantiotopic ligands and faces. Diastereotopic ligands and faces. Resolution -methods of Resolution.

Conformations six membered ring systems and their optical activity. Quantitative correlation between conformation and reactivity- Winstein-Eliel equation and Curtin-Hammett principle.

### Unit III: Reactive Intermediates & Methods of Determining Reaction Mechanism

Structure, stability, generation and reactions of Carbocations (classical and nonclassical), carbanions, carbenes, nitrenes and free-radicals.

Non-kinetic Methods - Product analysis and its importance-Intermediates and Transition states - Trapping, Testing and Detection of intermediates- Cross over experiments-. Isotopic labeling - Stereochemical studies. Kinetic methods: isotope effects: primary, secondary and solvent

isotope effect. Correlation Analysis - Linear free energy relationships - Hammett equation-significances of  $\sigma$  and  $\rho$ . □□ Applications of Hammett equation.

#### **Unit IV: Nucleophilic Substitutions in Aliphatic and Aromatic Substrates**

**Aliphatic nucleophilic substitution**  $S_N1$  and  $S_N2$  mechanisms-effect of substrate structure, leaving group, attacking nucleophile and solvent polarity-neighbouring group participation-substitution at vinylic and allylic carbons and reactivity. Ambient nucleophiles and substrates. Hydrolysis of esters-mechanisms. Selected reactions Von-Braun, Dieckmann, Williamson.

**Aromatic nucleophilic substitution** -  $S_NAr$  mechanism-  $S_N1$  (Aromatic) mechanism with evidences - Benzyne mechanism - Effect of substrate structure, leaving group, attacking nucleophile and solvent.

#### **Unit V: Selected topics for self study (Online)**

Strengths of acids and bases. Altermant and non-altermant hydrocarbons, Aromatic characterization of azulenes, tropones and annulenes. Racemization-methods-mechanisms of racemization through carbocations, carbanions and free-radicals. Conformations of mono and disubstituted three, four, five membered ring systems and optical activity. Conformations of decalin. Some selected reactions, Hunsdieker, Kolbe, Meerwein arylation, and Hofmann-Löffler-Freytag, Von Richter, Sommelet-Hauser and Smiles rearrangements.

Taft equation and its applications.

#### **TEXT BOOKS**

1. Cahn RS and Derner OC, *Introduction to Chemical Nomenclature*, Butterworth, London (1968).
2. March J, *Advanced Organic Chemistry*, Fourth Edition, John-Wiley and Sons, New York (1992).
3. Sykes P, *Guide Book to Mechanism in Organic Chemistry*, Sixth Edition, ELBS with Longmann (1997).
4. Eliel E L, *Stereochemistry of Carbon Compounds*, Tata-McGraw Hill Publishing Company, New Delhi (1998).

#### **REFERENCES**

5. Finar, I.L, *Organic Chemistry Volume 2*, Sixth Edition, ELBS with Longmann, Singapore (1997).
6. Nasipuri D, *Stereochemistry of Carbon Compounds*, Second Edition, New-Age International Publishers, New Delhi (1996).

Sem. I  
16PCH1103

Hours/Week: 6  
Credits: 5

## PHYSICAL CHEMISTRY-I

### Learning Assurances

- To understand the concepts and applications of reaction kinetics chemistry.
- To understand the concepts and applications of surface chemistry.
- To understand the electro analytical techniques, instrumentation and applications.

### Unit I: Theories of reaction rate (16 Hours)

Theories of reaction rates and reaction mechanism - Arrhenius equation - Potential energy surfaces and reaction coordinates - Collision theory - ARRT (thermodynamic and statistical treatments) - Application of ARRT to unimolecular, bimolecular and termolecular reactions - Kinetic isotope effect, isokinetic relation and temperature - Theories of unimolecular reactions - Lindemann and RRK - Principle of microscopic reversibility and detailed balancing.

### Unit II: Application of ARRT to solution kinetics ONLINE (16 Hours)

Application of ARRT to solution kinetics - Factors affecting reaction rate in solution-. Internal pressure - Solvent dielectric constant - Ionic strength - Hydrostatic pressure - Ion-dipole and dipole-dipole reactions - vant Hoff equation and volume of activation - Acid - base catalysis - vant Hoff and Arrhenius intermediates - Mechanism - protolytic and prototropic catalysis laws - Acidity functions - Hammett - Zucker hypothesis - Catalysis in biological systems. Michaelis - Menten equation - Lineweaver - Burk and Eadie - Hofstee plots -Influence of substrate concentration, pH, and temperature on rate - Influence of substituents on reaction rates - Hammett and Taft equations - Linear free energy relations.

### Unit III: Surface Chemistry, Heterogeneous Catalysis and Radiation Chemistry (16 Hours)

Surface phenomenon - Physical and chemical adsorption - Adsorption and free energy relations at interface - Langmuir adsorption isotherm - Gibbs adsorption isotherm-BET isotherm - Measurement of surface area - Heterogeneous catalysis - Mechanism - Langmuir - Hinshelwood Mechanism - Langmuir - Rideal bimolecular mechanism - Role of surface in catalysis - Radiation chemistry - Sources of high energy radiations - Interaction of high energy radiations with matter - Detection of radiations - Dosimeters - Primary and secondary processes. Radiolysis of water - Hydrated electron - G value.

### Unit IV: Debye - Huckel Theory and its Applications (16 Hours)

Debye Huckel theory - Radius of ionic atmosphere - Calculations of thickness of ionic atmosphere - Evidences of ionic atmosphere - Asymmetry effect - Electrophoretic effect - Debye Falkenhagen effect - Wien effect - Debye - Huckel Onsager equation - Modification and verification of the equation - Debye - Huckel limiting law - Modification and verification - Finite ion size model - Huckel -Bronsted equation - Calculation of activity coefficient - Determination of ion size parameter - solubility - solubility product of sparingly soluble salt - common ion effect - neutral salt effect and solubility - determination of solubility and solubility product.

**Unit V: Electrode Kinetics****(16 Hours)**

Theories of electrical double layer - Electric double layer at the electrode - electrolyte interface - Helmholtz model of double layer - Law of electro neutrality -Gouy-Chapman diffused charged model - Adsorption theory of double layer - Stern's model, triple-layer theory-. Electro capillary phenomenon - Electro capillary curves for solutions containing anions, cations and molecular substances - Electro capillary maximum – Lipmann equations and Lipmann potential - Experimental measurement and calculation of Lipmann potential - Capillary electrometer and contact angle method - Electro kinetic phenomena - Classification - Electro osmosis and electrophoresis - Streaming potential and sedimentation potential –Kinetics of electrode process - Equilibrium and non-equilibrium process - Concentration and activation polarization - Theory of electrochemical over potential - Derivation and verification of the equations - Butler – Volmer equation - Tafel equation.

**TEXTBOOKS**

1. Laidler K J, Chemical Kinetics, Third edition, New Delhi TATA McGraw Hill Co. (1984).
2. Kuriacose and Rajaram, Kinetics and Mechanism of Chemical Transformation, Macmillan & Co, Delhi (1993).
3. Glasstone S, An Introduction to Electrochemistry, New Delhi, East West Press Pvt. Ltd, (1956).

**REFERENCES**

1. Huges G, Radation Chemistry, Oxford series (1973).
2. Antorpov L, Theoretical Electrochemistry, Mirpublishers, Mascow.
3. Bockris J O'M and Reddy A K N, Modern Electrochemistry Vol 1 & 2, Second Edition, Plenum Press, New York (1998).

**Sem. I**  
**16PCH1104**

**Hours/Week: 4**  
**Credits: 3**

## **ORGANIC CHEMISTRY PRACTICAL-I**

### **Learning Assurances**

- Separation of binary organic mixtures
- Green Chemistry concepts
- Skills of doing microlevel analyses
- Methods of qualitative analysis of organic compounds
- Single stage preparation of organic compounds

### **1. Micro Qualitative Analysis of an organic binary mixture**

- i. Pilot separation
- ii. Bulk separation
- iii. Determination of melting and boiling points
- iv. Analysis of organic compounds
- v. Derivatization

### **2. Semi-micro Preparation of Organic compounds (single-stage and double stage)**

- i. Preparation of benzoic acid from toluene
- ii. Preparation of acetanilide from aniline
- iii. Preparation of p-nitro aniline from acetanilide
- iv. Preparation of p-bromo aniline from acetanilide
- v. Preparation of nitro methyl benzoate from methyl benzoate
- vi. Preparation of m-nitro benzoic acid from m-nitro methyl benzoate.

### **REFERENCES**

1. Furniss B S, Hannaford A J, Smith P W G and Tatchell A R, Vogel's Textbook of Practical Organic Chemistry- Fifth edition, Pearson publication.
2. Vengataswaran V et al., Basic Principle of Practical Chemistry – Sultan Chand and sons, New Delhi (1997).
3. Ganapragasm and Ramamurthy ,Organic Chemistry Lab Manual, Second Edition, S. Vishwanathan Printers and Publishers (P) Ltd., Chennai (2007).
4. Organic Chemistry Lab Manual for Micro Qualitative Analysis, Department of Chemistry, St. Joseph's College, Tiruchirappalli. (Private circulation)



**Sem. I**  
**16PCH1105**

**Hours/Week: 4**  
**Credits: 3**

### **PHYSICAL CHEMISTRY PRACTICAL-I**

#### **Learning Assurance**

- To learn some non-electrical physical chemistry experiments.
- To study the kinetics of some reactions.
- To learn the technique of developing phase diagram of some binary systems.
- To learn the determination methods of physical constants of substances.

#### **Regular Experiments**

1. Neutral salt effect - Kinetics of reaction between iodide and Persulphate - Effect of ionic strength on rate constant.
2. Polarimetry - Inversion of Cane sugar.
3. Kinetics of iodination of acetone.
4. Kinetics of hydrolysis of ester - Comparison of acid strengths.
5. Determination of Arrhenius parameters - Hydrolysis of methyl acetate by acid.
6. Partition coefficient - Study of  $KI + I_2 \rightleftharpoons KI_3$ .
7. Phase diagram of naphthalene - m-dinitrobenzene system. (Simple eutectic system).
8. Heat of fusion of naphthalene.
9. Heat of solution of oxalic acid by solubility.
10. Partial molar volume of electrolytes.
11. Freundlich's Adsorption Isotherm - Adsorption of acetic acid by charcoal.
12. Phase diagram of two-component system forming a compound.

#### **Demonstration experiments**

1. Kinetic study under low temperature with ultra crystal circulator.
2. Phase diagram of three-component system.

#### **REFERENCES**

1. Venkateswaran V, Veeraswamy R, Kulandaivelu A.R., Basic Principles of Practical Chemistry, (2nd edition), New Delhi, Sultan Chand & sons (1997).
2. Daniels et al., Experimental Physical Chemistry, (7th edition), New York, McGraw Hill (1970).
3. Findlay A, Practical Physical Chemistry, (7th edition), London, Longman (1959).

**Semester I**  
**16PPH1401**

**Hours : 4**  
**Credit : 4**

### **IDC-1(WS) : PHYSICS FOR COMPETITIVE EXAMS**

#### **Assurance of Learning**

The students will learn the following after going through this course

- Basic principles of physics
- Competitive examination skills
- Sharpen the thought process toward the objective type questions

#### **Unit – I: GENERAL MECHANICS AND PROPERTIES OF MATTER**

Physical quantities, SI system of units, Dimensions, Scalars and Vectors ( Concepts), Newton's Equations of Motion, impulse, Principle of conservation of Linear momentum, Projectiles, Kepler's Laws, Newton's Law of Gravitation, acceleration due to gravity, Escape velocity, Angular momentum, banking of roads, simple harmonic motion, Viscosity, Surface Tension

#### **Unit – II: HEAT AND THERMODYNAMICS**

Different scales of temperatures, thermal expansions, Calorimetry – specific heat, latent heat, triple point, transmission of heat, heat conductivity, Black bodies, Stefan Boltzmann Law, Wien's Displacement Law, Gas Equation, Boyle's Law, Charle's Law, Law of equipartition of energy

#### **Unit – III: LIGHT AND SOUND**

Reflection, Refraction and total internal reflection of light and their applications, propagation of light, Refractive index, Prism, Lenses, mirrors, Aberration in Lenses, Optical instruments – microscopes, telescopes, binoculars, Defects of Human Eye

Wave motion, longitudinal and Transverse waves, velocity of sound- Newton's formula, Laplace correction, effects of pressure - beats , laws of vibrating strings, open and closed organ pipes, Resonance

#### **Unit – IV: ELECTRICITY AND MAGNETISM**

Electric charge, field, potential, Resistances, Capacitance , cells and their combinations, Kirchoff's laws, Ohm's law, Faraday's laws, Lenz's law, Galvanometer, Voltmeter, Ammeter, Current Electricity.

Earth's Magnetism, bar magnet, Magnetic moment, Magnetic field, magnetic substances, torque of a bar magnet placed in a magnetid field, electromagnet.

#### **Unit – V: MODERN PHYSICS AND ELECTRONICS**

Bohr's theory, H spectrum, Nuclear Physics, Binding Energy, X – rays, Alpha, Beta and Gamma rays, Einstein's photo electric effect and mass-energy relations

Semi-conductors, Diodes, Transistors, Rectifiers, Amplifiers, Oscillators, Boolean Algebra, Logic gates, Electronics in Communication.

#### **BOOK FOR STUDY :**

Physics for Competitive Exams - Department of Physics , St. Joseph's College, Tiruchirappalli-2

INORGANIC CHEMISTRY – II

*Assurance of Learning*

- Concepts of ionic bonding and covalent bonding are learnt
- Acid base concepts are learnt
- Periodicity of elements and the chemistry of halogens and noble gases are learnt

**UNIT I: Ionic Bonding** (16 Hours)

Effective nuclear charge – shielding - Slater's rule – Born-Lande equation – Born Haber cycle and its applications – Radius ratio – polarization- Fajan's rule – results of polarization. Electronegativity – determination – methods of estimating charges, electronegativity equalization – Types of chemical forces – effects of chemical forces - melting and boiling points, solubility and hardness

**Unit II: Covalent Bonding** (16 Hours)

Valence bond theory – resonance – conditions of resonance – formal charge – hybridization – Molecular orbital theory – symmetry and overlap – molecular orbitals in homonuclear diatomic molecules: O<sub>2</sub>, B<sub>2</sub>, N<sub>2</sub> and C<sub>2</sub> – MO treatment of hetero nuclear diatomic molecules: CO and HCl – MO treatment of triatomic molecules such as BeH<sub>2</sub>. VSEPR theory: methane, ethylene, acetylene, ammonia, water, PCl<sub>3</sub>F<sub>2</sub> (Bent's rule), SF<sub>4</sub>, BrF<sub>3</sub>, TeF<sub>5</sub>, ICl<sub>2</sub><sup>-</sup>, ICl<sub>4</sub><sup>-</sup>, XeF<sub>2</sub>, XeF<sub>4</sub>, XeF<sub>6</sub>, XeO<sub>3</sub>, XeO<sub>4</sub>, XeO<sub>2</sub>F<sub>2</sub>, XeOF<sub>4</sub>, phosphorus trihalides, ammonia and NX<sub>3</sub> dipole moments, OF<sub>2</sub> and COF<sub>2</sub>. Bond angle - *s*, *p* character relationship – energetics of hybridization

**UNIT III: Acids and Bases** *ON-LINE* (16 Hours)

Electrode potentials and electromotive forces – applications – Acid-base concepts: Bronsted-Lowry, Lux-Flood, Usanovich, Lewis, solvent system and generalised acid base concepts – Measures of acid-base strength – steric effect and solvation effects *F*-strain and *B*-strain – Hard and soft acids and bases – acid base strength - hardness and softness – symbiosis –Theoretical basis of hardness and softness, electronegativity and hardness and softness Types of solvents, types of reactions – autoionisation, neutralisation, precipitation, solvation, solvolysis and complex formation. *Liq.* NH<sub>3</sub>, *liq.* SO<sub>2</sub>, HF and H<sub>2</sub>SO<sub>4</sub> as solvents - alkali metals in *liq.* NH<sub>3</sub>

**UNIT IV: Periodicity and the chemistry of halogens and noble gases** (16 Hours)  
**Periodicity**

The use of *p*-orbitals in *pi*-bonding – *pπ-pπ* bonding in heavier non-metals – the use of *d* orbitals by non-metals – experimental evidence of *pπ-dπ* bonding – comparison of *pπ* bonding in phosphine complexes and oxides – experimental evidences for *d*-orbital contraction and participation

**Chemistry of halogens and noble gases**

Interhalogen compounds – polyhalide ions – oxyacids of heavier halogens – anomalous behaviour of fluorine – structure and reactivity of noble gas fluorides

**Unit V: Inorganic chains, rings, cages and clusters****(16 Hours)**

Silicate minerals – *ortho*-, *pyro*-, and *meta*-silicates – pyroxene, amphiboles – two-dimensional silicates – talc, mica and three dimensional aluminosilicates, feldspar, zeolites, ultramarine – Silicones-preparation, properties and uses - Iso and hetero-polyacids Structures of  $[\text{TeMo}_6\text{O}_{24}]^{6-}$  and  $[\text{Mo}_7\text{O}_{24}]^{6-}$  ions and  $[\text{PMo}_{12}\text{O}_{40}]^{3-}$  ion – Polymeric sulphur nitride – borazines, phosphonitrilic compounds-trimers and tetramers - homocyclic inorganic ring systems – Concept of multi-centered bond – structure of  $\text{B}_2\text{H}_6$ ,  $\text{B}_4\text{H}_{10}$ ,  $[\text{B}_{12}\text{H}_{12}]^{2-}$ ,  $\text{B}_6\text{H}_{10}$ ,  $\text{B}_8\text{H}_{12}$ ,  $\text{B}_{10}\text{H}_{14}$ , Wade's rules, *closo*, *nido*, *arachno* boranes and carboranes and “*styx*” code.

**TEXTBOOK**

1. Huheey J E, Keiter E A and Keiter R L, *Inorganic Chemistry Principles of Structure and Reactivity*, 4e, Harper Collins College Publishers, New York, 1993

**REFERENCES**

1. Cotton F A and Wilkinson G, *Inorganic Chemistry A Comprehensive Text*, 3e, Interscience Publishers, New York, 1972
2. Purcell K F and Kotz J C, *Inorganic Chemistry*, W B Saunders Company, Philadelphia, 1977
3. Shriver D, Weller M, Overton T, Rourke J and Armstrong F, *Inorganic Chemistry* 6e, W H Freeman and Company, New York, 2014
4. Miessler G L, Fischer P J and Tarr D A, *Inorganic Chemistry*, 5e, Pearson Education, Inc., New York, 2014
5. Housecroft C E and Sharpe A G, *Inorganic Chemistry* 4e, Pearson Education Limited, Essex, 2012
6. Lee J D, *Concise Inorganic Chemistry*, 6e, ELBS, London, 1998

Sem: II  
Code: 16PCH2107

Hours: 6  
Credits: 5

## ORGANIC CHEMISTRY II

### Learning Assurance:

After learning these topics the students have sufficient knowledge on the following:

1. Electrophilic Substitution reactions in Aromatic and Aliphatic Substrates
2. The mechanisms addition, elimination, rearrangements, reductions and oxidation reactions
3. Some illustrative oxidising and reducing reagents and their characteristic reactions

### UNIT I: Electrophilic substitutions in Aromatic and Aliphatic Substrates

**Aromatic electrophilic substitution** - Arenium ion mechanism-Selected reactions - Reactivity-Nitration- Nitrosation - Sulphonation - Halogenation - Friedel Craft's reaction, Gattermann reaction- Vilsmeier Haack reaction - Gattermann Koch reaction- Reimer Tiemann reaction-Jacobsen reaction.

**Aliphatic electrophilic substitution** -  $S_E1$  and  $S_E2$  and  $S_Ei$  mechanisms-effect of substrate structure, leaving group, attacking nucleophile and solvent polarity. Selected reactions - Migration of double bonds-halogenation of aldehydes and ketones.

### Unit II : Addition and Elimination Reactions

Addition to carbon-carbon multiple bonds-addition mechanisms-electrophilic, nucleophilic and free-radical additions-cyclo addition-orientation and reactivity. Selected reactions - Birch reduction- Diels-Alder reaction- Hydroboration- Michael reaction.

Addition to carbon-hetero atom multiple bonds. Addition mechanisms-orientation and reactivity. Selected name reactions - Acyloin ester condensation reaction, Benzoin, Darzen's, Knoevenagel, Mannich, and Stobbe.

$E_1$ ,  $E_2$  and  $E_{1cB}$  mechanisms-spectrum of  $E_1$ ,  $E_2$  and  $E_{1cB}$  mechanisms, orientation and reactivity. Bredt's rule. Selected reactions-dehydration of alcohols-dehydrohalogenation-Chugave reaction- Cope elimination-Shapiro reaction. Extrusion Reactions

### Unit III: Oxidation and Reduction reactions

**Oxidations:** Weingberg Scheme of redox reactions -Synthetic uses of the following oxidants - DDQ, PCC, PDC, Jones reagent and chromyl chloride,  $MnO_2$ ,  $SeO_2$ ,  $KBrO_3$ , Thallium nitrate,  $OSO_4$ ,  $RuO_4$  Lemieux-Johnson reagents, Prevost woodward reactions,

**Reductions:** Dehydrogenating reagents, Bio-oxidants- catalytic hydrogenation-Synthetic uses of the following reductants  $NaNH_2$ , Wilkinson's catalyst,  $NaBH_4$ ,  $(t-BuO)_3AlH$ ,  $NaBH_3CN$ ,  $R_3SnH$ ,  $Me_3SiCl$ , alkali metals (Na, Li) Mg-Hg, hydrazine.

## UNIT V: Molecular Rearrangements and Name Reactions

Classifications-mechanisms and applications of the following rearrangements: Baeyer--Villiger, Beckmann, Curtius, Dienone-Phenol, Favorskii, Fries, Lossen, Neber, Schmidt, Stevens, Tiffenev-Demjanov ring expansion, Bamford-Stevens reaction.

### UNIT V : Selected topics for self study (Online)

Bischler Napieralski reaction-Pechman reaction- Houben-Hoesch reaction. Stork-Enamine reaction-decarboxylation of aliphatic acids-Haloform reaction, Aldol condensation, Cannizaro reaction, Claisen reaction, Hofmann exhaustive methylation, Oxidising reactions of  $\text{KMnO}_4$ ,  $\text{CrO}_3$ ,  $\text{Pb}(\text{OAc})_4$ , peracids, ozone, periodate, Reducing reactions - MPV reduction, Clemmenson reduction, Wolf-Kishner reduction.

### TEXT BOOKS

1. March J, *Advanced Organic Chemistry*, Fourth Edition, John-Wiley and Sons, New York (1992).
2. Sykes P, *Guide Book to Mechanism in Organic Chemistry*, Sixth Edition, ELBS with Longmann (1997).
3. Gould E S, *Mechanism and Structure in Organic Chemistry*, Holt-Reinhart and Winston, New York (1959).
4. Eliel E L, *Stereochemistry of Carbon Compounds*, Tata-McGraw Hill Publishing Company, New Delhi (1998).

### REFERENCES

1. Clayden, creaver, warren and wothers, *organic chemistry*, oxford University Press, New York (2006)
2. Final I L, *Organic Chemistry Volume I and II*, Sixth Edition, ELBS with Longmann, Singapore (1997)

## PHYSICAL CHEMISTRY – II

### Learning Assurance

- To study the fundamentals and applications of classical mechanics.
- To study the fundamentals and applications of quantum chemistry.
- To understand the symmetry of molecules and its applications.

### Unit I: Classical Mechanics (16 Hours) : ONLINE

Conservation Principles-- conservation of linear momentum, angular momentum and energy. Equations of motion - Newtonian, Lagrangian and Hamiltonian . Failure of Classical mechanics - Black body radiation , Photo electric effect , Heat capacity of substances , Hydrogen atomic spectrum. Wave particle dualism, de Broglie equation ,Compton effect, uncertainty principle and its applications, Conversion of classical wave equation into Schrodinger wave equation.

### UNIT II: Mathematics for Quantum Chemistry (16 Hours)

Functions - definition, classification, Linearly dependent and independent functions, odd and even functions. Inner product , Normalization , Orthogonality , orthonormal functions, Kronecker delta , proper function - Eigen functions - need for normalization. Review of vectors and vector spaces. Operators – Linear and non-linear operators. Commutation relationship, Construction of operators-Linear momentum, angular momentum and energy operators , commutation relation among angular momentum operators, Hermitian operators and their properties, anti Hermitian , Postulates of quantum mechanics.

### UNIT III: Basic Quantum Chemistry (16 Hours)

Solution of the Schrodinger equation for exactly solvable problems-Particle in a 1D and 3D boxes, Harmonic oscillator and Rigid rotor, Tunneling ,one dimensional potential barrier and wells, Solution of the Schrodinger equation for the hydrogen atom, Radial and angular probability distributions, Atomic orbitals and electron spin, Pauli's exclusion principle.

### UNIT IV: Rudiments of Group Theory (16 Hours)

Principles of Group theory-Symmetry elements - symmetry operations- Properties of group - Abelian, non - Abelian and cyclic groups-Multiplication Tables - Classes - subgroups-. Molecular point groups - Schoenflies symbols - Matrices for symmetry operations - Reducible and irreducible representations - Statement of Great Orthogonality theorem – Construction of character Table - Explanation of a character Table.

### UNIT V: Applications of Group Theory (16 Hours)

Applications of Group theory - Standard reduction formula relating reducible and irreducible representations - Hybridization schemes for atoms in molecules of different geometry - AB<sub>4</sub> tetrahedral, AB<sub>3</sub> triangular planar. Symmetries of vibrational modes in non-linear molecules (H<sub>2</sub>O, NH<sub>3</sub> and BF<sub>3</sub>) - Integration method - Selection rules in spectroscopy – IR & Raman active – Vibrational modes - Mutual exclusion rule - Symmetry in crystals - Hermann - Mauguin symbols- . Space groups of crystals - Translational elements of symmetry – Comparison of crystal symmetry with molecular symmetry

### REFERENCES

1. Prasad R K, *Quantum Chemistry*, V Edition, New Delhi, Wiley Eastern Ltd, (1992).
2. Anderson J M, *Mathematics of Quantum Chemistry*, First Edition, Massachusetts, W.A. Benjamin Inc. (2005)
3. Donald A McQuarrie, *Quantum Chemistry*, Indian Edition, Viva Books Private Ltd. (2007)
4. Gupta and Kumar, *Classical Mechanics*.
6. Levine I N, *Quantum Chemistry*, sixth Edition, Prentice Hall of India, Pvt. Ltd (2009).
7. Atkins P W, *Molecular Quantum Mechanics*, Clarendon (1973).
8. Raman K V, *Group Theory and its Applications to Chemistry*, New Delhi, TATA McGraw Hill Co, (1990).

## ORGANIC CHEMISTRY PRACTICAL-II

### Learning Assurances

- Quantitative analysis in organic chemistry
- Double stage organic preparations
- Chromatographic techniques

#### 1. Quantitative Analysis

- i. Determination of saponification value of oil.
- ii. Estimation of iodine value of oil.
- iii. Estimation of phenol and aniline.
- iv. Estimation of ketone.
- v. Estimation of glucose.
- vi. Estimation of nitrogen by Kjeldhal method.
- vii. Estimation of Ascorbic acid.

2. Rotary flash evaporation technique.

3. Paper chromatography.

4. Thin layer chromatography.

5. Column chromatography.

### REFERENCES

1. Furniss BS, Hannaford AJ, Smith PWG, Tatchell AR, *Vogel's Textbook of Practical Organic Chemistry*, Fifth edition, Pearson publication.
2. Vengataswaran V et al., *Basic Principle of Practical Chemistry*, Sultan Chand and sons, New Delhi (1997).
3. Ganapragasm and Ramamurthy, *Organic Chemistry Lab Manual*, Second Edition, S.Vishwanathan Printers and Publishers (P) Ltd., Chennai (2007).



## PHYSICAL CHEMISTRY PRACTICAL-II

### Learning Assurance

- To learn some electro analytical experiments.

### Experiments

1. Determination of Copper and Nickel by electro gravimetry.
2. Determination of standard electrode potential of Zinc and Copper.
3. Polarographic determination of Zinc ion and Cadmium ion.
4. Salting out constant - Effect of NaCl on solubility of Benzoic acid.
5. Dissociation constant of weak acid by conductivity method.
6. Determination of second-order rate constant for saponification of ethyl acetate by conductivity.
7. Conductometric acid-base titration - mixture of acids - dibasic acid.
8. Conductometric precipitation titration - iodide and chloride mixture.
9. Potentiometric precipitation titration - mixture of iodide, bromide and chloride versus silver nitrate.
10. Solubility of sparingly soluble salt by (i) Conductivity and (ii) Potentiometry.
11. Determination of equivalent conductance of a strong electrolyte at infinite dilution.
12. Potentiometric Redox titration.

### Demonstration Experiments

- Measurement of dipole moment with dipole meter.
- Measurement of ultrasonic velocity by ultrasonic interferometer.

### REFERENCES

1. Venkateswaran V, Veeraswamy R., Kulandaivelu A.R., *Basic Principles of Practical Chemistry*, Second edition, New Delhi, Sultan Chand & sons, (1997).
2. Daniels *et al.*, *Experimental Physical Chemistry*, Seventh edition, New York, McGraw Hill, (1970).
3. Findlay A, *Practical Physical Chemistry*, Seventh edition, London, Longman (1959).

**Self-Paced Learning: NATURAL PRODUCTS****Learning Assurances**

- Structure, reactions and biological functions of biomolecules are learnt
- Preparation methods and reactions of the five, six and fused heterocyclics were studied
- Nature, structure, isolation, classification, functions and structural elucidation of natural products were studied

**UNIT I Carbohydrates****(12 Hours)**

Carbohydrates – Ring structures – Fischer's proof for the configuration of D(+) glucose – Citric acid cycle – Structure of fructose, sucrose, maltose, lactose and cellobiose – Structural difference between starch and cellulose

**UNIT II Proteins and Nucleic acids****(12 Hours)**

Amino acids – Synthesis of amino acids Proteins (Strecker synthesis and Gabriel synthesis) – Peptides and peptide synthesis (Merrifield resin synthesis) – End group analysis – structure of proteins – primary, secondary, tertiary and quaternary.

**Nucleic acids**

Nucleic acids – nucleosides and nucleotides in nucleic acids – structure and biological implications of DNA and RNA (*m*-RNA, *t*-RNA and *r*-RNA)

**UNIT III Alkaloids, Terpenoids and Antibiotics****(12 Hours)**

**Alkaloids:** Introduction – extraction – classification – structural elucidation of papaverine only.

**Terpenoids:** Introduction – extraction – classification – structural elucidation of Zingiberene only.

**Antibiotics:** Structure-activity relationship of chloramphenicol – structure and functions of penicillin, streptomycin and terramycin.

**UNIT IV Hormones (Online)****(12 Hours)**

Hormones – Introduction – chemical nature – Prostaglandins-structure and formation (structural elucidation not required). Structural elucidation of cholesterol (synthesis not required). Sex hormones – Structure and properties of oestrone, equilinin, androsterone, testosterone (elucidation not required).

**UNIT V Heterocyclics****(12 Hours)**

Preparation, physical properties and reactions of five-membered and six-membered heterocyclics containing one hetero atom (pyrrole, furan, thiophene and indole, pyridine, quinoline and isoquinoline). Only the structures and numbering and naming of diazines (pyrazine, pyrimidine and pyrazine), azines (oxazine and azepine).

**Textbook**

1. Finar I L, *Organic Chemistry* Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997).

**Reference**

2. Jayashree Gosh, *Textbook of Pharmaceutical Chemistry*, S. Chand & Chand publications New Delhi (1997).

**Sem. II**  
**16PSS2401**

**Hours/Week: 4**  
**Credits: 4**

**IDC: SOFT SKILLS**

### INORGANIC CHEMISTRY-III

#### *Assurance of Learning*

- Theories of bonding in coordination compounds are learnt
- Kinetics and mechanisms of reactions of complex compounds are learnt
- Physical methods in the study of complex compounds are learnt

#### **UNIT I: Theories of Coordination Chemistry (16 Hours)**

Crystal field theory – Splitting pattern of octahedral, tetrahedral, square planar, trigonal bipyramidal and square pyramidal complexes – Magnetic properties, CFSE, high spin-low spin cross over – limitations – Structural and thermodynamic effects of inner orbital splitting, Jahn-Teller effect (static, dynamic, elongation and flattening) – Ligand Field theory – Evidences for M-L overlap, spin-orbit coupling constant and Racah parameters – MO theory of Octahedral complexes (sigma and pi bonding) – MO of tetrahedral and square planar complexes.

#### **UNIT II: Basics of Organometallics (16 Hours)**

Types of ligands – hapticity – isolobal concept – 16 and 18 electron rules – applications and limitations – Carbonyls – bonding – terminal, doubly, triply bridged carbonyls – structure of carbonyls – CO stretching frequencies of carbonyls and mixed carbonyls – Carbonyl hydrides – Nitrosyls: terminal, bridging and bent – *Pi* complexes with olefins – ferrocene and benzenoid metal complexes – Nonbenzenoid aromatics as ligands and carbene complexes – fluxional molecules

#### **UNIT III: Reaction Kinetics in Coordination Chemistry *ON-LINE* (16 Hours)**

Inert and labile complexes – Stepwise, overall stability constants – Chelate effect – Mechanisms – Associative, Interchange associative, Dissociative, Interchange dissociative –  $S_N1$ ,  $S_N2$ , Solvent intervention, ion pair formation and  $S_N1CB$  – evidences – Acid and base hydrolysis – mechanisms and evidences – Trans effect – theories and Applications – Electron transfer reactions – inner and outer sphere mechanisms – remote and adjacent attacks – Catalysis by organometallic compounds – oxidative addition – insertion – hydrogenation (Wilkinson's catalyst) – hydroformylation – Wacker process – Fischer-Tropsch reaction – Zeigler-Natta Catalyst

#### **UNIT IV: Physical Methods in Coordination Chemistry–I (16 Hours)**

Types of magnetic behaviour – magnetic susceptibility measurements – Gouy method – Orbital contribution – Spin-orbit coupling and its effects on magnetic properties – Temperature independent paramagnetism (TIP) – Electronic spectra of complexes – bandwidth and intensity – Sugano-Tanabe and Orgel Diagrams – charge transfer spectra – Infrared spectra of Coordination complexes – characteristic frequencies – mode of coordination and interpretation of  $ClO_4^-$ ,  $SO_4^{2-}$ ,  $CO_3^{2-}$ , ester, amine, amide, DMSO and urea using IR spectra

## UNIT V: Physical Methods in Coordination Chemistry–II

(16 Hours)

NMR – Applications of NMR to inorganic compounds – NMR of metal hydrides ( $^1\text{H}$  NMR), metal carbonyls( $^{13}\text{C}$  NMR),  $^{19}\text{F}$  and  $^{31}\text{P}$  NMR – ESR – zero-field splitting – Kramer's degeneracy – pattern for number of lines of complexes having  $d^1$ - $d^9$  systems – bis(salicylaldimine) Cu(II), Mn(II) complexes – Mossbauer spectroscopy – quadrupole interactions – magnetic interactions –  $\text{FeSO}_4$ ,  $\text{FeCl}_3$ , ferro- and ferricyanides, nitroprusside,  $\text{Fe}_3(\text{CO})_{12}$ ,  $\text{I}_2\text{Br}_2\text{Cl}_4$

### TEXTBOOKS

1. Cotton F A and Wilkinson G, *Inorganic Chemistry A Comprehensive Text*, 3e, Interscience Publishers, New York, 1972
2. Huheey J E, Keiter E A and Keiter R L, *Inorganic Chemistry Principles of Structure and Reactivity*, 4e, Harper Collins College Publishers, New York, 1993
3. Drago R S, *Physical Methods in Chemistry*, 3e, W. B. Saunders Company, London, 1992

### REFERENCES

1. Purcell K F and Kotz J C, *Inorganic Chemistry*, W B Saunders Company, Philadelphia, 1977
2. Shriver D, Weller M, Overton T, Rourke J and Armstrong F, *Inorganic Chemistry* 6e, W H Freeman and Company, New York, 2014
3. Miessler G L, Fischer P J and Tarr D A, *Inorganic Chemistry*, 5e, Pearson Education, Inc., New York, 2014
4. Housecroft C E and Sharpe A G, *Inorganic Chemistry* 4e, Pearson Education Limited, Essex, 2012
5. Lee J D, *Concise Inorganic Chemistry*, 6e, ELBS, London, 1998
6. Lewis J and Wilkins R G, *Modern Coordination Chemistry*, Interscience Publishers, Inc., New York, 1960
7. Sutton D, *Electronic Spectra of Transition Metal Complexes*, McGraw Hill, Australia, 1968
8. Basalo F and Pearson R G, *Mechanisms of Inorganic Reactions*, John-Wiley and Sons Inc., New York, 1960
9. Crabtree R H, *The Organometallic Chemistry of the Transition Metals*, 6e, John-Wiley and Sons Inc., New York, 2014
10. Kazuo Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part A and B, 6e, John-Wiley and Sons, Inc. New York, 2009
11. Straughn B P and Walker S, *Spectroscopy* Volumes 1, 2 and 3, Chapman and Hall, London, 1976
12. Ebsworth EAV, *Structural Methods in Inorganic Chemistry*, 3e, Great Britain, ELBS, 1987
13. Parish R V, *NMR, NQR, EPR, and Mossbauer Spectroscopy in Inorganic Chemistry*, Ellis Harwood Limited, London, 1990
14. Gibbs T C, *Principles of Mossbauer Spectroscopy*, Chapman and Hall, London, 1976

**SEM: III**  
**Code: 16PCH3113**

**Hours: 6**  
**Credits: 5**

### **ORGANIC CHEMISTRY - III**

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#### **Learning Assurances:**

- The principle, instrumentation and applications of various spectroscopic techniques are learnt.
  - The basics and applications of synthetic organic chemistry are learnt.
  - The principle, stereochemistry and applications of photochemistry and Pericyclic reactions are understood.
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#### **UNIT I: Organic Spectroscopy - I**

UV-Visible spectroscopy-Electromagnetic spectrum – Energy-Wavelength Relationship- basic principles of electronic transitions-correlation of electronic transitions-differentiating geometrical and positional isomers-Some terms: chromophore, auxochrome - Woodward-Fischer rules applied to conjugated dienes,  $\alpha$  and  $\beta$  -unsaturated carbonyl compounds & aromatic systems.

IR spectroscopy-Hooke's Law-types of vibrations - characteristic group frequencies and factors influencing them- -inter and intra molecular hydrogen bonding-conformational aspects in cyclic 1, 2- and 1, 3- diols - Finger print region- applications of IR.

#### **UNIT II: Organic Spectroscopy – II**

PMR spectroscopy-principle-Magnetically active nuclei - Number of signals – Position of signals (chemical shift)- Peak area and proton counting- magnetic non equivalence of protons-- types of coupling and coupling constants ( $J^1$ ,  $J^2$  - values) -correlation of chemical shift with structure-spin decoupling of exchangeable protons-. CMR spectroscopy - Basic principles-broad band and off-resonance decoupling – NOE, DEPT - ESR spectroscopy-predicting number of ESR lines for simple organic free radicals such as methyl, ethyl, phenyl, naphthyl radicals.

#### **Unit III: Organic Spectroscopy - III**

Mass spectrometry - basic principles-parent, base and meta stable peaks- calculation of molecular formula-Nitrogen rule–McLafferty rearrangement-fragmentation pattern of various classes of organic compounds

Joint applications of UV -Visible, IR, NMR and mass spectrometric methods to structural elucidation of organic compounds

#### **UNIT IV Organic Synthetic Methods (Online)**

Synthons and synthetic equivalents-types of synthons - umpolung reactions-typical examples. Retrosynthetic analysis-designing syntheses by disconnection approach. Formation of carbon-heteroatom bonds. Ring opening and ring closure reactions. Regioselective and stereoselective alkylation-cyclic ketones - cyclic enones- 1, 3-diketones- $\beta$ -keto esters- $\alpha$ -halo ketones. C versus O alkylation - enamines and selective alkylation Protecting groups- protection of hydroxyl, carboxyl, carbonyl and amino groups-illustration of protection and deprotection in syntheses.

## **UNIT V: : Photochemistry and Pericyclic reactions – Online**

Photochemistry - Fundamental concepts-Joblanskii diagram-photosensitization. Photochemical reactions – photoaddition - photoreduction - photooxidation - photochemical rearrangements - Norrish type-I and type - II reactions - Paterno-Buchi reaction - Barton reaction. Di-*pi* methane rearrangement. Photochemistry of alkenes, dienes, carbonyl compounds and aromatic compounds.

Pericyclic reactions - Characteristics-types-applications of FMO and MO correlation diagram methods to electrocyclic and cycloaddition reactions- Woodward-Hoffmann rules and their applications to simple systems-cycloadditions involving hydrogen transfer-Sigmatropic reactions-Cope and Claisen rearrangements-

### **TEXTBOOK**

1. Kemp W, *Organic Spectroscopy*, Third Edition, ELBS, London (1987).
  2. Stewart Warren, *Designing Organic synthesis: The Disconnection Approach*, Wiley, New Delhi, (1984)
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### **REFERENCES:**

1. March J, *Advanced Organic Chemistry*; Fourth Edition, John-Wiley and Sons, New York (1992).
  2. Silverstein R M and Bassler G C, *Spectrometric Identification of Organic Compounds*, Fourth Edition, John- Wiley and Sons, New York (1993).
  3. Fleming I, *Spectroscopic Methods in Organic Chemistry*, Fourth Edition, Tata-McGraw Hill Publishing Company, New Delhi (1988).
  4. Clayden, Greaver, Warren and Wothers, *Organic Chemistry*, Oxford University Press, New York (2006).
  5. Morrison R. T. and Boyd R. N., *Organic Chemistry*, Sixth Edition, Allyn & Bacon Ltd., New York (1976)
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**Sem. III**  
**16PPS3101**  
**Common Core:**

**Hours/Week: 6**  
**Credits: 5**

## **METHODS OF SPECTROSCOPY AND LASERS**

### **Learning Assurance**

- To understand the basic concepts of molecular spectroscopy.
- To study in detail Raman and electronic spectroscopies.
- To study in detail NMR, NQR and ESR spectroscopies.

### **UNIT-I:**

#### **Rotational and Vibrational Spectroscopy**

**(16 Hours)**

Basic aspects of Spectroscopy-characterisation of electromagnetic radiation, quantization of energy. Microwave Spectroscopy-Rotation of molecules and selection rules, Diatomic molecules; Rigid and nonrigid rotor, Rotational constant and centrifugal distortion. Techniques and instrumentation. Vibrational spectroscopy-diatomic molecules, Harmonic and anharmonic oscillators, zero point energy - force constant - fundamental absorption and overtones (hot bands, fermi resonance)- polyatomic molecules-techniques and instrumentation of FTIR.

### **Unit II:**

#### **Raman and NMR spectroscopy**

**(16 Hours)**

-Raman spectroscopy - Raman and Rayleigh scattering - Quantum and classical theories of Raman effect - Pure rotational Raman spectra – Stokes and anti-stokes lines - Vibrational Raman spectra-Mutual exclusion rule - Polarised and depolarized Raman lines - Techniques and instrumentation. NMR - Hydrogen nuclei - Chemical shift and spin - spin splitting – Coupling constant ( $J$ ). Splitting with and without chemical exchange-instrumentation- Interaction between spin and magnetic field - Gyromagnetic ratio - FT NMR.

### **UNIT III:**

#### **ESR spectroscopy**

**(16 Hours)**

ESR-Principle-Position of ESR absorptions -  $g$  value - Hyperfine splitting -Zero field splitting - ESR spectrum of free radicals and copper salicylaldehyde complexes. Mossbauer spectroscopy - principles of Mossbauer spectroscopy, Doppler shift, recoil energy, isomer shift, quadrupole splitting- applications to various compounds.

### **UNIT IV:**

#### **Electronic Spectroscopy**

**(16 Hours)**

Electronic spectra - Electronic spectra of diatomic molecules - Born - Oppenheimer approximation- vibrational coarse structure- Franck – Condon Principle-, Dissociation energy and dissociation products - rotational fine structure of electronic vibration -vibration transition - Fortrate Diagram. Electronic angular momentum in diatomic molecules-spectrum of Molecular hydrogen - Molecular photoelectron spectroscopy - UV photo electron spectroscopy and X-ray photo electron spectroscopy.



## **UNIT V:**

### **Laser devices and their Applications**

**(16 Hours)**

Principle - pumping He-Ne laser Carbon dioxide laser, semi conductor laserholography recording and reconstruction-applications laser induced fusion process- stimulated Raman scattering laser in isotope separation lidar-laser tracking- lasers in industry and medicine.

## **REFERENCES**

1. Banwell C N, *Molecular spectroscopy*, New Delhi, TATA McGraw Hill Co. (1997).
2. Drago R S, *Physical Methods in Inorganic Chemistr*, New Delhi, East West Press Ltd, (1971).
3. Chang R, *Basic Principles of Spectroscopy*, New Jersy, Englewood Cliffs (1978).
4. Straughan B P and Walker S, *Spectroscopy Volume 1,2,3*, New York, London Chapman and Hall, A Halstet Press Book, John Wiley & Sons Ins. (1975).
5. Barrow G M, *Introduction to Molecular Spectroscopy*, Tata McGraw - Hill Edition (1993).
6. Gurdeep R Chatwal and Sham K Anand, *Spectroscopy*, Himalaya Publishing House (2009).

**Sem. III**  
**16PCH3114**

**Hours/Week: 4**  
**Credits: 3**

**INORGANIC CHEMISTRY PRACTICAL-I**

*Assurance of Learning*

- Qualitative analysis of common metals and rare metals are practiced
- Colorimetric estimation of some metal ions are done

**Experiments**

1. Systematic qualitative analysis of mixtures containing 4 cations of which 2 are rare.
2. Colorimetric estimation of iron, copper, nickel and manganese.

**REFERENCES**

1. Svehla G, *Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis*, 5e, Longman, London, 1979
2. Ramanujam V, *Inorganic Semi-micro Qualitative Analysis*, 3e, National Publishing Company, Chennai, 1990

Sem. III  
16PCH3202A

Hours/Week: 4  
Credits: 4

**Core Elective-2A: THERMODYNAMICS-I**

**Learning Assurance**

- To understand the fundamental and applications of statistical thermodynamics.
- To understand the fundamental and applications of partial molar properties.
- To study the basics and applications of chemical thermodynamics.
- To study the instrumental techniques used in chemical thermodynamics.

**UNIT I: Fundamentals of Statistical Thermodynamics (12 Hrs)**

Statistical method- Microstates, macro states - Permutations and combinations- Combinatory rule - probability theorems. –Ensembles- Phase space-Thermodynamic probability- Statistical equilibrium- Maxwell-Boltzmann statistics -Derivation of M.B. statistics-Relationship between entropy and probability- Heat capacity of solids- Einstein and Debye models-Statistical meaning of third law of thermodynamics.

**UNIT II: Applications of Statistical Thermodynamics (12 Hrs)**

Partition functions – molar, translational, rotational and vibrational partition functions of diatomic and polyatomic molecules-separation of partition function according to forms of energy-partition function and vibrational energy-total partition function-Electronic partition function-Derivation of thermodynamic quantities E, S, A, H, G, K and  $C_p$ ,  $C_v$  using partition function-Sackur-Tetrode equation- Bose Einstein statistics- -Fermi Dirac statistics- Electronic heat capacity of gases-equipartition of energy-classical and quantum statistical theory of heat capacities-heat capacities for diatomic molecule-rotational heat capacity of hydrogen molecule-Nuclear spin statistics-nuclear spin entropy- Quantum statistics.

**UNIT III: Chemical Thermodynamics I (12 Hrs)**

**Partial molar properties** – molarity and mole fraction –partial molar quantities-Methods of determination of partial molar volume- Chemical potential - Gibbs-Duhem equation -Chemical potential of mixture of gases - Chemical potential in terms of U, H - Variation of chemical potential with temperature and pressure – determination of partial molar properties from apparent molar properties-Free energy of mixing, entropy of mixing and volume of mixing. **Fugacity** - Definition-Methods of determination - Variation of fugacity with temperature, pressure and composition - Duhem-Margules equation - Fugacity of solids, liquids and mixture of gases - Determination of fugacity in gas mixtures (Lewis-Randall Rule).

**UNIT IV: Chemical Thermodynamics II and Numerical Problems in Thermodynamics (12 Hrs):**

**Activity** – activity and activity coefficients - Definition - Standard state, reference state, choice of standard state for gases, liquids and solids, liquid solvent and solute – dependence of activity on temperature and pressure-Determination of activity coefficient of non electrolyte – Mean ionic activity - Determination of activity coefficient of electrolytes by freezing point method.

**Laws of thermodynamics**- I law and II law of thermodynamics based on Reversible isothermal process of ideal and real gases – Irreversible isothermal process of ideal and real gases-Reversible adiabatic process of ideal and real gases - Irreversible adiabatic process of ideal and real gases- problems in I and II laws of thermodynamics.

**UNIT V: Chemical Thermodynamics III****ONLINE****(12 Hrs)**

Joule Thomson effect- Thermo chemistry - Kirchoff's equation- III law of thermodynamics - Determination of  $\Delta H$  by Bomb Calorimeter – Determination of density and viscosity of liquids and liquid mixtures-Determination of volume of mixing by relative density method- Ultrasonic interferometer and its application..

**TEXTBOOK**

1. Kuriakose J.C and Rajaram J.C, *Thermodynamics*, Jalandar Shoban Lal Co., (1999).

**REFERENCES**

1. Gupta M.C, *Statistical Thermodynamics*, second edition, New Age International Publishers, Chennai (1998).
2. Francis W. Sears and Gerhard L. Salinger, *Thermodynamics, Kinetic theory and statistical Thermodynamics*, Third edition, Narosa Publishing House, Chennai(1998).
3. Glasstone S, *Thermodynamics for Chemists*, New Delhi, East West Affiliated Pvt. Ltd, (1969).
4. Donald McQuarrie, *Statistical Thermodynamics*, Indian Edition, Viva Books Private Ltd., New Delhi (2003).
5. Ferrell L Hill, *Introduction to Statistical Thermodynamics*, Addison- Wesley Publishing Company, INC, London (1962).
6. Web resources and e- content.

**Sem. III**  
**16PCH3202B**

**Hours/Week: 4**  
**Credits: 4**

**Core Elective-2B: THERMODYNAMICS-II**

**Learning Assurance**

- To study the basics and applications of chemical thermodynamics.
- To understand the basics and applications of non- equilibrium thermodynamics.
- To understand the basics and applications of phase equilibria.
- To study the instrumental techniques used in chemical thermodynamics.

**UNIT I**

**(12 Hrs)**

Introduction to non equilibrium thermodynamics - Methods of study of non-equilibrium thermodynamics- Mass conversion de- Donder equation- Energy conservation-Entropy production in systems involving heat transfer - Entropy production in chemical reactions -Affinity and equilibrium constant.

**UNIT II**

**(12 Hrs)**

Affinity and Gibbs free energy - Affinity and rate derivations - Coupled and non coupled reaction systems - Entropy production and entropy flow in open system - Onsager Theory -Phenomenological relations - an introduction - Characteristics of direct and cross coefficients - Rate expression using Onsager equation - Kinetic approach - Thermodynamic approach – Derivation of Onsager reciprocity relation using a cyclic coupled reaction (Proof of  $L_{12} = L_{21}$ ).

**UNIT III**

**(12 Hrs)**

Linear law - Condition for coupled and non coupled reactions with reference to cross coefficients - Decomposition of cyclohexane and linear law – Non coupled reaction -Isomerization of xylene - Coupled reaction – Reaction taking place in liver - Experimental verification of Onsager's reciprocity relation - Thermoelectricity - Seebeck effect - Peltier effect - Electro kinetic effect - Thermo molecular pressure difference -  $L_{12} = L_{21}$  by transference number method - Irreversible thermodynamics and biological systems.

**UNIT IV**

**(12 Hrs)**

Phase equilibrium - phase rule - one, two and three component systems - Water, sulphur, carbon dioxide, lead - silver, KI - water, benzene - naphthalene, ferric chloride - water and acetic acid - chloroform – water-. Colligative properties.

**UNIT V:**

**ONLINE**

**(12 Hrs)**

Experimental methods used in thermodynamics - Determination of  $\Delta H$ ,  $\Delta S$ ,  $\Delta G$  - determination of heat of mixing and volume of mixing – Adiabatic compressibility (ultrasonic interferometer) - Bomb Calorimeter – Vapour pressure by isoteniscope method- sonochemistry and sonochemical reactions.

**TEXTBOOK**

1. Kuriakose J.C and Rajaram J.C, *Thermodynamics*, Jalandar Shoban Lal Co., (1999).

**REFERENCES**

1. Gupta M.C, *Statistical Thermodynamics*, second edition, New Age International Publishers, Chennai (1998).
2. Francis W. Sears and Gerhard L. Salinger, *Thermodynamics, Kinetic theory and statistical Thermodynamics*, Third edition, Narosa Publishing House, Chennai(1998).
3. Glasstone S, *Thermodynamics for Chemists*, New Delhi, East West Affiliated Pvt. Ltd, (1969).
4. Donald McQuarrie, *Statistical Thermodynamics*, Indian Edition, Viva Books Private Ltd., New Delhi (2003).
5. Ferrell L Hill, *Introduction to Statistical Thermodynamics*, Addison- Wesley Publishing Company, INC, London (1962).
6. Web resources and e- content.

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**IDC (BS): HEALTH CHEMISTRY**

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**Learning Assurances**

After learning these topics, the students will have sufficient knowledge on the following:

1. the importance of health and functions of drugs
2. the functions of enzymes, hormones and body fluids
3. causes of common diseases and their treatment

**UNIT I . Health and its Maintenance**

Definition: Food, Food Pyramid - Health-Hygiene- mal-, under- and over- nutrition, their causes and remedies, sanitation, Carbohydrates – Classification and their Biological functions, Proteins- Classification and their Biological functions, vitamins – Classification and their Biological functions

**UNIT II . Drugs and their Functions**

Drugs - Types of drugs and their functions- analgesics, antipyretics, antibiotics, antiseptics and disinfectants, depressants and anti-depressants, narcotics, muscle relaxants and cardiovascular agents and anticonvulsants.

**UNIT III . Body fluids**

Blood volume, Blood groups, Functions of blood, blood pressure, anemia, blood sugar, hemoglobin- chemistry of respiration-urine-electrolyte balance

**Unit IV. Enzymes, Hormones, Digestion**

Types of enzymes and enzyme action, Characters of hormones- action, examples of essential hormones - digestion in mouth, stomach, intestine and pancreas.

**UNIT V. Common Diseases**

**ONLINE**

Toxicants in food- cancer-types and causes- common diseases - Jaundice, vomiting, fever, rickets, scurvy, beriberi, pellagra, night blindness, ulcer, gout, goiter, diabetes.

**TEXT BOOKS**

1. Alex V Ramani, Food Chemistry, MJP Publishers, Chennai, 2009
2. Deb A C, *Fundamentals of Biochemistry*, New Central Book Agency, Calcutta, 1994.
3. Satake M and Mido Y, *Chemistry for Health Science*, Discovery Publishing House, New Delhi, 2003.
4. Jayashree Ghosh, *A Text book of Pharmaceutical Chemistry*, S. Chand and Co.Ltd, 1999.

**REFERENCE**

1. Ashutosh Kar, Medicinal Chemistry, Wiley Easterns Limited, New Delhi, 1993

Sem. IV  
16PCH4115

Hours/Week: 4  
Credits: 4

## INORGANIC CHEMISTRY-IV

### Assurance of Learning

- Structures of various solid inorganic molecules are learnt
- Chemistry of crystalline defects and their effects were learnt
- Importance of inorganic species in biological processes are learnt

### UNIT I: Solid State –I

(12 Hours)

Elements of crystallography – space lattices-unit cell – crystal systems – X-ray diffraction Bragg's method – Rotating crystal method and powder methods – indexing of crystal planes – Structure of typical lattices such as sodium chloride, cesium chloride, zinc blende, wurzite, rutile, fluorite, antiferite, perovskite and  $\text{ReO}_3$

### UNIT II: Solid State –II

(12 Hours)

Spinel and anti-spinel – Applications of CFT – covalent crystals diamond and graphite –Crystal Structure and properties – Types of solids – stoichiometric defects – point, line and plane defects – colour centers – nonstoichiometric defects –  $n$ ,  $p$  semiconductors – structure of solids – free electron and band theory of solids – Electrical conductivity and superconductivity – high temperature superconductors

### UNIT III: Photochemistry ON-LINE

(12 Hours)

Laws of photochemistry – Photo physical processes – Jablonski diagram – Fluorescence – Phosphorescence – Kasha's rule – Stoke's shift – Types of electronic transitions in transition metal complexes – *Photo chemistry of transition metal complexes* – Photo substitution – Photo aquation – Adamson's rules – Photo rearrangement – Photo redox reactions – *Photo chemistry of organo metallic compounds*.

### Unit IV: Bio-inorganic Chemistry–I

(12 Hours)

Structure and function of chlorophyll - Role of  $\text{Mg}^{2+}$  ion- Structure and function of Haemoglobin - Cooperative effect in Haemoglobin - Role of Globin - Structure and function of Myoglobin - Structure and function of Cytochrome C.

### UNIT V: Bio-inorganic Chemistry–II

(12 Hours)

Structure and function of Blue copper proteins – Structure and function of Vitamin  $\text{B}_{12}$  – *In-vivo* nitrogen fixation – Fe-S proteins – Ionophores – Ion transport mechanism in cell membrane – Na-K pump – Role of metal ions in DNA replication, transcription, translation – Role of *cis*-platin in the treatment of cancer

### TEXTBOOKS

1. Bertini I, Gray H B, Lippard S J and Valentine J S, *Bioinorganic Chemistry*, University Science Books, California, 1994
2. Tuli G D, Madan R D, Basu S K and Satya Prakash, *Advanced Inorganic Chemistry Volume I and II*, S. Chand & Company Ltd, 2014

### REFERENCES

1. Azaroff, *Introduction to Solids*, Tata McGraw Hill Publishing Co., New Delhi, 1994
2. Evans R C, *Crystal Chemistry*, Cambridge University Press, London, 1964
3. Addison W E, *Structural Principles of Inorganic Compounds*, Longman, London, 1961
4. West A R, *Solid State Chemistry and its Applications*, 2e, John-Wiley and Sons Ltd., New York, 2014
5. Keer H V, *Principles of Solid State*, Wiley Eastern Ltd, New Delhi, 1993
6. Wheatly P J, *The Determination of Molecular Structure*, Oxford University Press, London, 1959
7. Rohatgi-Mukherjee K K, *Fundamentals of Photochemistry*, New Age International Publishers, New Delhi, 2006

SEM: IV  
Code:16PCH4116

Hours: 4  
Credits: 4

## ORGANIC CHEMISTRY IV

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### Learning Assurances:

- The 12 principles of Green chemistry and its application in synthesis are studied.
  - The basics and application of organometallics and electro-organic methods in organic synthesis are learnt.
  - The stereochemistry aspects- asymmetric synthesis are learnt.
  - The fundamentals of electroorganic synthesis are known.
- 

### Unit I: Green Chemistry

**Green Chemistry:** The 12 principles, atom economy for addition, elimination, substitution reactions and its calculation, green starting materials, green reagents, green catalysts and green reactions.

### UNITII: Electro Organic Chemistry

Electro organic Reactions - Basic requirements for conducting electro-organic syntheses - Effects of variables-Reduction of carbonyl, nitro and carbon-halogen bonds-oxidation of unsaturated compounds-electro initiated polymerization.

### Unit III: Organometallics in Organic Synthesis

Introduction-Formation of organometallics (Mg, Li) - Oxidative insertion of Mg and Li into alkyl halides, deprotonation of alkyne, ortholithiation of functionalized benzene rings, halogen metal exchange, transmetallation – Applications –

Chan-Lam Coupling, Hiyama coupling - Corey-Fuchs Reaction,  $\text{Me}_2\text{CuLi}$  (Gillman's reagent), Heck reaction, Suzuki coupling, Stille coupling, Sonogashira reaction, Fukuyama Coupling - Negishi Coupling, Kumada Coupling.

### Unit IV: *Asymmetric Synthesis and Name Reactions*

Nucleophilic addition to chiral carbonyl compounds, by chiral reagents: Chirally modified LAH and BINAL-H, by chiral auxiliaries derived from Valine, by chiral catalyst, by alkylation of carbonyl compounds, by chiral Michael addition -. Uses of special reagents containing B, P and Si. Baylis-Hillman reaction – Biginelli reaction – Mukaiyama aldol reaction – Prins reaction, Mitsunobu reaction – Weinreb ketone synthesis Henry reaction – Hosomi-Sakurai reaction.

### Unit V: Organic Synthesis & Reactions - A Review (Online)

Synthetic applications of organozinc, organocadmium reagents.

**Olefination** of carbonyl compounds: McMurry's polyolefination, Peterson synthesis, Eglinton reaction, Wittig reaction and modifications. Phase transfer catalysis-crown ethers. Merrifield resin synthesis.

Routine functional group transformations and inter conversions of simple functionalities. Problems involving prediction of products of organic reactions-Problems in proposing mechanisms of organic reactions-Assigning reagents for organic reactions- introducing and inter converting functional groups in organic compounds-Problems involving transformation of organic compounds.



## TEXTBOOK

1. Paul T Anastas and John C Warner, *Green Chemistry: Theory and Practice*, Oxford University Press, UK (1998).
2. Jonathan Clayden, Nick Greevs, Stuart Warren and Peter Wothers , *Organic chemistry*.

## REFERENCES:

1. Paul T Anastas, *Text Book on Green Chemistry*, OUP, (2006).
2. March J, *Advanced Organic Chemistry*; Fourth Edition, John-Wiley and Sons, New York (1992).
3. Paula yurkanis Bruice, *Organic Chemistry*, Seventh Edition, Prentice Hall (2013).
4. Finar I L, *Organic Chemistry* Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997).
5. Mendham J, Denney R C, Barnes J D and Thomas M J K, *Vogel's Textbook of Quantitative Chemical Analysis*, Sixth Edition, Pearson Education, New Delhi,( 2000).

**Sem. IV**  
**16PCH4117**

**Hours/Week: 4**  
**Credits: 4**

### **INORGANIC CHEMISTRY PRACTICAL-II**

#### ***Assurance of Learning***

- Quantitative separation of metal ions in binary mixtures are learnt
- Simple single stage preparations of some complex compounds were learnt
- Characterization methods of complexes were learnt

#### **Experiments**

1. Quantitative analysis of a mixture of iron (volumetry) and copper (gravimetry)
2. Quantitative analysis of a mixture of copper (volumetry) and nickel (gravimetry)
3. Quantitative analysis of a mixture of iron (volumetry) and zinc (gravimetry)
4. Quantitative analysis of a mixture of copper(volumetric) and zinc (gravimetry)
5. Preparation of any three complexes
6. Determination of  $m_{eff}$  of a complex by Gouy method (internal evaluation only)
7. IR interpretation of a complex to find out the mode of coordination (internal evaluation only)
8. Interpretation of electronic spectrum of a complex (internal evaluation only)

#### **REFERENCES**

1. Jeffery G H, Bassett J, Mendham J and Denney R C, Vogel's *Textbook of Quantitative Chemical Analysis*, 5e, Longman Scientific & Technical, Essex, 1989
2. Department Material, St. Joseph' College (Autonomous), Tiruchirappalli

**Sem. IV**  
**16PCH4118**

**Hours/Week: -**  
**Credits: 2**

**COMPREHENSIVE EXAMINATION**

Sem. IV  
16PCH4202A

Hours/Week: 4  
Credits: 4

### Core Elective-IIA: PHYSICAL CHEMISTRY-III

#### Learning Assurances

- To know the importance of emf measurement
- To study the various electro analytical techniques, instrumentation and applications.
- To understand the concepts and applications of quantum chemistry.

#### Unit I: ONLINE

##### EMF Measurements and Applications

(12 Hours)

EMF and thermodynamics quantities - Nernst equation - Gibb's Helmholtz relation and EMF - Reversible electrodes - Types- electrode potentials - single electrode potential - electrochemical series - chemical cells - concentration cells with and without transference- Applications of EMF measurements - Activity coefficients and solubility determination- Storage and Fuel cells.

#### Unit II:

##### Electro analytical Techniques - I

(12 Hours)

Polarography - Experimental set up - Advantages of dropping mercury electrode Supporting electrolyte - Maxima suppressor - Residual current - Migration current -Diffusion current - Polarogram, half wave potential - Ilkovic equation (derivation is not required) - Outline of applications (Polarogram of  $Zn^{2+}$  and  $Cd^{2+}$ )-Cyclic voltametry, Principle, Experimental set up - Cyclic voltammogram of  $Fe^{2+}$  in  $H_2SO_4$  - Anodic peak current - Cathodic peak current - Electrochemically reversible couple - Cathodic peak potential - Electrochemically irreversible couple - Outline of applications.

#### UNIT III:

##### Electro analytical Techniques II

(12 Hours)

Amperometry - Principle of amperometric titration - Different types of current - voltage curves - Amperometric titration between  $Pb^{2+}$  and  $K_2Cr_2O_7$  Electrogravimetry, Principle, Experimental set up - Physical characteristics of metal deposits Separation of Cu & Ni - Coulometry, Principle, Experimental set up - Controlled potential coulometric analysis and application - Experimental set up for constant current Coulometry - Coulometric titration of Fe(II) with Cerium(III).

#### UNIT IV:

##### Applications of Quantum Chemistry-I

(12 Hours)

Approximation methods - Need for approximation - Perturbation Theory - Time independent Perturbation (First order only) - Application of Perturbation theory to particle in one dimensional box, anharmonic oscillator and helium atom - Principle of variation and its proof, trial function and secular determinant- Variation methods and its applications to hydrogen and helium atoms, particle in one dimensional box.

## UNIT V:

### Applications of Quantum Chemistry-II

(12 Hours)

The Born - Oppenheimer approximation , VB theory of hydrogen molecule and MO theory of hydrogen molecular ion ( $H_2^+$ ) - coulomb integral, exchange integral and overlap integral, Detailed calculation of energy and overlaps .Construction of sp, sp<sup>2</sup> and sp<sup>3</sup> hybrid orbitals , Huckel molecular orbital theory- principles and applications to ethylene, butadiene , benzene, cyclobutadiene,trimethylenemethane,bicyclobutadiene and allyl systems . Hartree-Fock method, self consistent field method and derivation of Hartree fock ,Roothan equations

### TEXTBOOKS

1. Willard, Merit, Dean and Settle, *Instrumental Methods of Analysis*, CBS Publication (1986). Delhi (1992).
2. Anatharaman R, *Fundamentals of Quantum Chemistry*, McMillan, New Delhi (2001).
3. Prasad R K, *Quantum Chemistry*, Wiley Eastern Ltd, New Delhi (1992)
4. Donald A McQuarrie, *Quantum Chemistry*, Indian Edition, Viva Books Private Limited (2007).

### REFERENCES

1. Vogel A I, *Text book of Quantitative Inorganic Analysis* ELBS (1978).
2. I.N.Levine, *Quantum chemistry*, Sixth edition, PHI Learning Private Limited,(2009)
3. Noel M and Vasu K I , *Cyclic voltammetry and the Frontiers of Electrochemistry*, Oxford and IBH (1990).
4. Kissinger P T and Heinman, *Laboratory Techniques in Electroanalytical Chemistry*, Editors, Marcel Dekker, Inc., New York (1984).

**Sem. IV**  
**16PCH4202B**

**Hours/Week: 4**  
**Credits: 4**

**Core Elective-IIB: POLYMER CHEMISTRY**

**Learning Assurance**

- To understand the basic concepts of polymer chemistry.
- To study the stereochemical, morphological and other properties of polymers
- To study in detail the applications and kinetics of polymerization techniques.

**UNIT – I:**

**Introduction to Polymer Science** **ONLINE** **(12 Hrs)**

Polymer science-History - Concepts and terminology. Classification of polymers (with suitable examples) based on origin, structure, backbone, branching, action of heat, ultimate form and use, crystalline and amorphous behaviour Ladder, semi-ladder and spiro polymers. Molecular forces in polymers - dipole forces, induction forces, dispersion forces, H-bond. Dependence of physical properties on intermolecular forces. Monomers, structure and main features of some common polymers and polyurethane elastomers. Inorganic polymers: Types of inorganic polymers, preparation, structure and properties of polyphosphazenes, polysiloxanes, polysilanes, polygermanes and polystannanes.

**UNIT – II:**

**Stereochemistry and Conformation of Polymers** **(12 Hrs)**

Constitutional isomerism-positional isomerism and branching, substitutional isomerism (with suitable examples). Configuration and conformation of macromolecules: stereoisomerism-optical isomerism and geometrical isomerism, configuration of polymer chains-stereoregular polymers, tacticity in polymers-motactic and ditactic polymers. Experimental and spectroscopic methods for the determination of configuration, conformation of single macromolecule, conformation in the crystal, micro conformation in solution, ideal coil molecules in solution, compact molecules. Optically active poly(olefins), poly(amino acids), proteins. Conformational transitions.

**UNIT – III:**

**Morphology and Order in Crystalline Polymers** **(12 Hrs)**

Polymer morphology: common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallizability mechanism of crystallization Polymer single crystals: lamellar structure of polymers-fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model. Structure of polymers: crystallized from melt-super crystalline structures, spherulitic morphology, mechanism of spherulite formation. Theories of crystallization, kinetics- Avrami equation, Hoffman's nucleation theory, the entropic barrier theory. Strain induced morphology, cold drawing, morphology changes during orientation. Theory and application of XRD, SEM and DSC in determining the crystallinity of polymers.

#### **UNIT – IV:**

##### **Polymer Solutions (12 Hrs)**

Solubility of low molecular weight substances and polymers. Theories of polymer solubility, different stages of polymer solubility, non solvents, solubility of amorphous and crystalline polymers, solubility parameter concept. Thermodynamics of polymer solution: lattice theory- advantages and limitations of lattice theory, Flory-Huggins and Flory-Krigbaum theories - advantages and limitation of FH and FK theories, corresponding state theories, Flory temperature, polymer - solvent interaction parameter, the unperturbed polymer chain, expansibility factor, entropy, enthalpy and free energy of mixing of polymer solution, phase separation in polymer systems. The models of De Gennes and Edwards tube model (worm model), self avoiding random walk, scaling concepts in polymer systems, pearl model.

#### **UNIT – V:**

##### **Kinetics of Polymer Chemistry (12 Hrs)**

Kinetics of polymerization - Free radical polymerization – Cationic polymerization - Anionic polymerization - Emulsion polymerization - Number average molecular weight of polymers - Molecular weight by Cryoscopy, ebullioscopy, Osmotic pressure method - Average molecular weight determination - Light scattering method - Using ultra centrifugation by sedimentation equipment - Sedimentation velocity - Differential scanning calorimetry - Differential thermal analysis - Thermo gravimetric analysis - Models of viscoelastic behaviour - Hooke model - Newton model - Voigt model - Burger Maxwell model - Kelvin - Voigt model - Glass transition temperature - Measurement of T<sub>g</sub> - molecular interpretation of T<sub>g</sub>.

#### **REFERENCES**

1. Gowariker V R, Viswanathan N V, Sreedhar J, *Polymer Science*, New Age International (2011).
2. Billmeyer F W Jr., *Text book of Polymer Science*, Third Edition, John Wiley & Sons (1984).
3. Sperling LH, *Introduction to Physical Polymer Science*, Fourth Edition, Wiley-Inter science (2005).
4. Cowie JMG, Arrighi V, *Polymers: Chemistry and Physics of Modern Materials*, Third Edition, CRS Press (2007).
5. Bower DI, *An Introduction to Polymer Physics*, Cambridge University Press (2002).
6. Chanda M, *Introduction to Polymer Science and Chemistry, A Problem Solving Approach*, CRS Press (2006).
7. Flory PJ, *Principles of Polymer Chemistry*, Cornell University Press (1953).
8. de Gennes P G, *Scaling Concepts in Polymer Physics*, Cornell University Press (1979).
9. Teraoka, *Polymer Solutions: An Introduction to Physical Properties*, John Wiley & Sons, (2002).
10. Chandrasekhar V, *Inorganic and Organometallic Polymers*, Springer (2005).

Sem. IV  
16PCH4203A

Hours/Week: 4  
Credits: 4

### Core Elective-III A: ANALYTICAL CHEMISTRY

#### *Assurance of Learning*

- Nature of errors and their types are learnt
- Statistical methods in error analysis are learnt
- The theory, instrumentation, types and applications of chromatographic techniques are learnt
- Methods of thermal analyses are studied

#### UNIT I: ERROR ANALYSIS - I

Significant figures – rounding off the values – accuracy and precision – errors – classification of errors – constant errors and proportional errors – determinate errors (systematic errors) and indeterminate (random and accidental) – minimization of errors: calibration of apparatus, analysis of standard samples, running a blank determination, and independent analysis.

#### UNIT II: ERROR ANALYSIS - II

Average, range, median, average deviation, relative average deviation and standard deviation, variance, coefficient of variation – the normal error curve – testing of significance: *F*-test, *t*-test and *Q*-test – confidence limit – method of least squares

#### UNIT III: THERMOANALYTICAL METHODS AND COLORIMETRY

General Characteristics of thermoanalytical methods – Thermogravimetric analysis – Principle, instrumentation and applications – Factors affecting thermogram – Differential Thermal Analysis- DTA instrumentation and applications – Differential scanning calorimetry – Principle, instrumentation and applications

Colorimetry – fundamental laws – deviations from Beer's law – instrumentation and applications of spectrophotometry

#### UNIT IV: INSTRUMENTAL METHODS OF ANALYSIS

Principle, instrumentation and applications of fluorimetry, phosphorimetry

Flame photometry and atomic absorption spectrophotometry – Theory, instrumentation, interferences and applications.

#### UNIT V: CHROMATOGRAPHY *ON-LINE*

Principles of chromatography – retardation factor – plate theory – column efficiency – Classification of chromatographic techniques – Principle, instrumentation and applications of gas chromatography (GC), thin-layer chromatography (TLC) and high-performance liquid chromatography (HPLC)

#### TEXTBOOK

1. Jeffery G H, Bassett J, Mendham J and Denney R C, *Vogel's Textbook of Quantitative Chemical Analysis*, 5e, Longman Scientific & Technical, Essex, 1989

#### REFERENCES

1. Gary A Christian, *Analytical Chemistry*, 6e, John Wiley & Sons Inc., 2004
2. Gopalan R, Subramanian P S, Rengarajan K, *Elements of Analytical Chemistry*, 3e, Sultan Chand & Sons, New Delhi, 2003
3. Skoog D A, Holler F J and Crouch S R, *Principles of Instrumental Analysis*, 6e, Thompson Brooks/Cole, Belmont CA, 2007
4. Skoog D A, West D M, Holler F J and Crouch S R, *Fundamentals of Analytical Chemistry*, 9e, Brooks/Cole, Belmont CA, 2014



**Sem. IV**  
**14PCH4203B**

**Hours/Week: 4**  
**Credits: 4**

**Core Elective-IIIB: PHARMACEUTICAL CHEMISTRY**

**Learning Assurances**

- Design, structure and structure activity relationship of drugs are learnt
- Various modes of spread of common diseases and their treatment are learnt
- Advanced drugs for new diseases are learnt

**Unit-I: Introduction to Chemistry of Drugs (12 Hours)**

Drugs - definition- sources- study of drugs -classification (Biological chemical, commercial and utility)-Nomenclature of drugs- Biotransformation- Drug design - factors affecting the stability of drugs- Encapsulation – drug delivery systems and sustained release of drugs.

**Unit-II: Pharmaceutical Aids (12 Hours)**

Preservatives- Antioxidants- Sequestering agents- Emulsifiers- Colorantsm Flavoring agents - Sweeteners - Stabilizers- suspending agents- Ointment bases- Solvents.

**Unit-III: Common Diseases and Treatment (12 Hours)**

Insect borne diseases - Treatment using drugs - Air borne diseases- Treatment using drugs - water borne diseases- Treatment using drugs- Digestive disorders - treatment- diseases of respiratory system- treatmentdiseases of nervous system - treatment - Other common diseases- treatment.

**Unit-IV: Pathogenicidal Drugs (12 Hours)**

Antibiotics - Classification- Chloramphanicol- penicillin-streptomycin- Tetracycline - Macrolides-Erythromycin - Rifamycin- Antiseptics and disinfectants - Phenols Halogen compounds - Analgesics - Antipyretics - Anti -inflammatory agents - Sulpha drugs.

**Unit-V: Bio Regulatory Drugs (12 Hours)**

Cardiovascular drugs - Cardiac glycosides - anti arrhythmic drugs - antihypertensive agents - antianginal agents. Diabetes and Hypoglycaemic drugs - two types of diabetes - Insipidus and mellitus - Control of diabetes - Insulin -Hypoglycaemic agents. Anticonvulsants - Cancer and antineoplastic drugs - Common causes - antimetabolites.

**Reference**

1. Jayashree Gosh, *Textbook of Pharmaceutical Chemistry*, S. Chand & Chand Publications, New Delhi (1997)

**Sem. IV**  
**16PCH4501**

**Hours/Week: 10**  
**Credits: 5**

**DISSERTATION & VIVA VOCE**