

# University of Mumbai



## DEPARTMENT OF CHEMISTRY (AUTONOMOUS)

### INFORMATION BROCHURE FOR M. Sc. DEGREE PROGRAMMES IN INDUSTRIAL POLYMER CHEMISTRY

DEPARTMENT OF CHEMISTRY  
UNIVERSITY OF MUMBAI  
VIDYANAGARI  
SANTACRUZ (E)  
MUMBAI – 400 098

In Collaboration with



### Indian Rubber Manufacturers Research Association

An Autonomous Body under DPIIT, Min. of Comm. & Ind., Govt. of India

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**2021-2022**

**SYLLABI FOR M. Sc. CHOICE BASED CREDIT SYSTEM (CBCS) FOUR-  
SEMESTER-COURSE IN CHEMISTRY**

**SEMESTER-I**

Course Code	Title of the Course	No. of Credits	No. of hours per SEMESTER	Examination		Total Marks
				Mid Sem Marks	End-Sem Marks	
IPCHEM 101	Physical Chemistry I	4	60	40	60	100
IPCHEM 102	Inorganic Chemistry I	4	60	40	60	100
IPCHEM 103	Organic Chemistry I	4	60	40	60	100
IPCHEM 104	Analytical Chemistry I	4	60	40	60	100
IPCHEM 105	Physical Chemistry Practical I	2	-	-	50	50
IPCHEM 106	Inorganic Chemistry Practical I	2	-	-	50	50
IPCHEM 107	Organic Chemistry Practical I	2	-	-	50	50
IPCHEM 108	Analytical Chemistry Practical I	2	-	-	50	50
	Total	24			Total	600

**\* Practical component involves 16 h per week laboratory work for 15 weeks.**

## **SYLLABUS: SEMESTER-I**

### **IPCHEM 101: PHYSICAL CHEMISTRY-I**

#### **Unit-I-THERMODYNAMICS-I[15L]**

State function, exact and inexact differentials, Internal energy, Enthalpy, Heat capacity, Relation between  $C_p$  and  $C_v$ , Limitations of first law of thermodynamics, Joule-Thomson experiment, Joule-Thomson coefficient, Joule-Thomson coefficient for real and an ideal gas, Inversion temperature

Absolute temperature, Spontaneous or irreversible process, Entropy, Thermodynamic equation of state, Maxwell relation, Helmholtz and Gibbs free energy, Third law of thermodynamics, Nernst heat theorem, Determination of absolute entropies, entropy changes in chemical reaction, residual entropy.

#### **Unit-II-FUNDAMENTAL ASPECTS OF QUANTUM CHEMISTRY** [15L]

**Introduction:** Historical background, Old Vs New Quantum Theory, Heisenberg's Uncertainty Principle, The wave nature of matter

**Fundamental Background:** Postulates of Quantum Chemistry, Commutators of operators, Properties of Linear and Hermitian operators, Operators for the dynamic variables of a system such as position, linear momentum, angular momentum and total energy, Expectation Value,

Progressive and standing waves, Conditions on the wave function and its interpretation, Normalization and orthogonality, Separation of variables, Obtaining Schrödinger's time independent wave equation from Schrödinger's time dependent wave equation.

**Application of Quantum Chemistry in Translation motion:** Particle in one dimension box: Differential equation and its solution, Graphical representation of wavefunctions and probability densities, Normalization and orthogonality of wave functions. Even and Odd Functions.

Particle in a two and three dimensional box: Differential equation and its solution, Degeneracy, Energy level Diagram.

#### **Unit-III-PHASE RULE AND ITS APPLICATIONS** [15L]

Phase rule, Phase diagrams and their classification, Lambda transitions.

Two component system: Vapor pressure – composition diagrams, Phase diagrams for partially miscible liquids for two components, Critical solution temperature, influence of foreign substances on CST, fractional distillation of Zeotropic and Azeotropic mixtures.

Three component systems:

Type I-Formation of one pair of partially miscible liquids: Graphical representations, binodal curves, plait point, influence of temperature-System showing real critical solution temperature, System showing no real critical solution temperature.

Type II-Formation of two pairs of partially miscible liquids.

Type III-Formation of three pairs of partially miscible liquids, Influence of impurities, Ternary Azeotropic mixtures, Preparation of absolute alcohol by azeotropic elimination of water.

#### **Unit-IVCHEMICAL KINETICS [15L]**

Accounting for the rate laws: simple reactions, temperature dependence of reaction rates, consecutive reactions,(rate determining step approximation and steady-state approximation), unimolecular reactions – Lindemann-Hinshelwood mechanism.

Kinetics of complex reactions - Chain reactions, polymerization reactions, explosions, photochemical reactions.

Fast reactions: Study of kinetics by flow methods, relaxation methods, flash photolysis, magnetic resonance method, shock tube method.

***\*Derivation not expected***

***Note: Numerical and theoretical problems from each Unit- are expected.***

#### **References books:**

1. Peter Atkins and Julio de Paula, *Atkin's Physical Chemistry*, 7<sup>th</sup> ed., Oxford University Press, 2002.
2. K. J. Laidler and J. H. Meiser, *Physical Chemistry*, 2<sup>nd</sup> ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3<sup>rd</sup> ed., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5<sup>th</sup> ed., Tata McGraw-Hill, New Delhi, 2002.
5. G. W. Castellan, *Physical Chemistry*, 3<sup>rd</sup> ed., Narosa Publishing House, New Delhi, 1983.
6. D. A. McQuarrie and J. D. Simon, *Physical Chemistry - a molecular approach*, Viva Books Private Limited, New Delhi, 1998.
7. S. Glasstone, *Text Book of Physical Chemistry*, 2<sup>nd</sup> ed., McMillan and Co. Ltd., London, 1962.
8. D. A. McQuarrie, *Quantum Chemistry*, Viva Books Private Limited, New Delhi, first Indian ed., 2003.
9. B. K. Sen, *Quantum Chemistry including spectroscopy*, Kalyani Publishers, 2003.
10. A. K. Chandra, *Introductory Quantum Chemistry*, Tata Mc Graw-Hill, 1994.
11. R. K. Prasad, *Quantum Chemistry*, 2<sup>nd</sup> ed., New Age International Publishers, 2000.
12. D. O. Hayward, *Quantum Mechanics for Chemists*, Royal Society for Chemists, 2002.
13. Sydney T. Bowden, *The phase rule and the phase reaction*, McMillan and Co. Ltd., London, 1938.

14. A. N. Cambell, Alexander Findlay, *The Phase Rule and its Applications*, Dover publications.
15. G. L. Agarwal, *Basics Chemical kinetics*, Tata Mcgraw Hill, New Delhi.
16. K. J. Laidler, *Chemical Kinetics*, 3<sup>rd</sup> ed., Pearson Education.
17. R. P. Rastogi, R. R. Mishra, *An Introduction to Chemical Thermodynamics*, Vikas Publishing House Pvt. Ltd.

**List of Books for further reading:**

1. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
2. W. G. Davis, *Introduction to Chemical Thermodynamics – A Non-Calculus Approach*, Saunders, Philadelphia, 1972.
3. I. M. Klotz and R. M. Rosenberg, *Chemical Thermodynamics*, 5<sup>th</sup> ed., John Wiley and Sons, Inc., 1994.
4. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
5. Ira N. Levine, *Quantum Chemistry*, 5<sup>th</sup> ed., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
6. J. P. Lowe, *Quantum Chemistry*, 2<sup>nd</sup> ed., Academic Press, New York, 1993.
7. R. Anantharaman, *Fundamentals of Quantum Chemistry*, McMillan India Limited, 2001.
8. Mahendra R. Awode, *Quantum Chemistry*, S. Chand and Co. Ltd., New Delhi, 2002.

**IPCHEM-102: INORGANIC CHEMISTRY-I**

**Unit-I      INORGANIC REACTION MECHANISMS      [15L]**

- (i) Rate of reactions, factors affecting the rate of reactions; techniques for the determination of rate of reactions.
- (ii) Mechanisms and factors affecting the (I) ligand substitution reactions of (a) octahedral complexes with and without breaking of metal-ligand bond, (b) square planar complexes – trans-effect, its theories and applications and (c) tetrahedral complexes; (II) Redox reactions: inner and outer sphere mechanisms.
- (iii) Complimentary and non-complimentary reactions.
- (iv) Isomerization and racemization reactions.

**Unit--II      ORGANOMETALLIC CHEMISTRY      [15L]**

- (i) Recapitulation of classification of organometallic compounds, electron

counting and eighteen electron rule.

- (ii) Sixteen electron rule.
- (iii) Synthesis, structure and bonding of the following organometallic compounds:
  - (a) Alkyl and Aryl derivatives, (b) Carbenes and Carbynes, (c) Alkene complexes, (d) Alkyne complexes, (e) Allyl complexes, (f) Cyclopentadiene complexes and (g) Arene complexes (sandwich and half sandwich complexes).

### **Unit-III CHEMICAL BONDING**

[15L]

- (i) **Hybridization:** Derivation of wave functions for the following orbital hybridisation types:  $sp$  ( $\text{BeH}_2$ );  $sp^2$  ( $\text{BF}_3$ );  $sp^3$  ( $\text{CH}_4$ ) considering only sigma bonding.
- (ii) Molecular Orbital Theory (LCAO-MO approach) for Electron deficient and Electron rich species.
- (iii) Hydrogen bonding: concept, types, properties, methods of detection and importance. Van der Waal's forces, ion-dipole, dipole-dipole, London forces.
- (iv) Bent's Rule: Reactivity of molecules: e.g. chlorofluorides of phosphorous, fluoromethanes, etc.

### **Unit-IV CHEMICAL REACTIVITY**

[15L]

- (i) Hydration of cations and anions, Latimer equations, acidity of cations and oxocations, basicity of anions and oxoanions, classification of mono and polyatomic ions on the basis of  $pK_a$  with predominance diagram. Classification of oxoacids, structural anomalies.
- (ii) Recapitulation of hard soft acids and bases (HSAB) principle, Acid-base strength and softness and hardness; Classification of Lewis acids and bases based on frontier Molecular orbital topology, Reactivity matrix of Lewis acids and bases; Superacids and bases.
- (iii) Redox properties of the elements:
  - Latimer diagram: Construction of the diagram, non-adjacent species and disproportionation.
  - Frost Diagram: Construction and interpretation.
  - Pourbaix diagram of Iron in natural water.

### **Reference books:**

#### **Unit-I**

1. D. Banerjee, Coordination Chemistry, Tata McGraw Hill, 1993.
2. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2<sup>nd</sup>Ed., Wiley, 1967.
3. M. L. Tobe and J. Burgess, Inorganic Reaction Mechanism, Longman, 1999.
4. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry,

5<sup>th</sup>Ed., Oxford University Press, 2010.

5. R. Gopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd., 2001

### **Unit-II**

1. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 5<sup>th</sup>Ed., Wiley Interscience, 2009.
2. R. C. Mehrotra and A. Singh, Organometallic Chemistry-A Unified Approach, 2<sup>nd</sup>Ed., New Age International Pvt. Ltd., 2000.
3. G. O. Spessard and G. L. Miessler, Organometallic Chemistry, Prentice-Hall, 1977.
4. K. F. Purcell and J. C. Klotz, Inorganic Chemistry, Saunders, 1977.
5. B. Douglas, D. H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chemistry, 2<sup>nd</sup> Ed., John Wiley & Sons, 1983.
6. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4<sup>th</sup> Ed., Harper Collins, 1993.

### **Unit-III**

1. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4<sup>th</sup> Ed., Harper Collins, 1993.
2. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Oxford University Press, 1967.
3. R. L. Dekock and H.B.Gray, Chemical Structure and Bonding, The Benjamin Cummings Publishing Company, 1989.
4. K. L. Kapoor, A textbook of Physical Chemistry, Volume 4, McMillan, 2001.
5. G. Miessler and D. Tarr, Inorganic Chemistry, 3<sup>rd</sup> Ed., Pearson Education, 2004.
6. R. Sarkar, General and Inorganic Chemistry, Books & Allied (P) Ltd., 2001.
7. C. M. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 1985.
8. J. N. Murrell, S. F. A. Kettle and J. M. Tedder, The Chemical Bond, Wiley, 1978.
9. G. A. Jeffrey, An Introduction to Hydrogen Bonding, Oxford University Press, Inc., 1997.
10. W. W. Porterfield, Inorganic Chemistry-A Unified Approach, 2<sup>nd</sup> Ed., Academic Press, 1993.
11. B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.

### **Unit-IV**

1. G. Wulfsberg, Inorganic Chemistry, Viva Books Pvt. Ltd., 2002.
2. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup>Ed., John Wiley & Sons, Inc., 2001.
3. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5<sup>th</sup>Ed., Oxford University Press, 2010.
4. G. Miessler and D. Tarr, Inorganic Chemistry, 3<sup>rd</sup> Ed., Pearson Education, 2004.
5. B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.

6. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4<sup>th</sup> Ed., Harper Collins, 1993.
7. R. L. Madan and G. D. Tuli, Inorganic Chemistry, 5<sup>th</sup> Ed., S. Chand, 2012.
8. J. D. Lee, Concise Inorganic Chemistry, 5<sup>th</sup> Ed., Wiley, 2012.
9. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone, 2014.
10. <http://www.meta-synthesis.com/webbook.html>

### **IPCHEM 103: ORGANIC CHEMISTRY-I**

#### **Unit-IPHYSICAL ORGANIC CHEMISTRY [15L]**

##### **1.1 Acidity-Basicity:**

Different concepts and examples, Factors affecting acidity & basicity. Electrophilicity and Nucleophilicity; Ambident Electrophiles and Nucleophiles, Relationship between nucleophilicity and basicity.

##### **1.2 Non-kinetic Methods of determining reaction mechanism:**

Product profiles, Detection and identification of intermediates by chemical/trapping and spectroscopic means. Evidence from catalysis, cross-over experiments, isotopic labeling, Kinetic isotope effect-primary & secondary isotope effect, Stereochemical studies.

##### **1.3 Linear Free Energy Relationships:**

Effect of structure on reactivity, Hammett equation, substituent and reaction constants, Through conjugative effects of substituents, Linear free energy relationships in the determination of reaction mechanism, Taft Equation, steric parameter.

#### **Unit-II STEREOCHEMISTRY [15L]**

##### **2.1: Symmetry operations and symmetry elements:**

Symmetry Operations, identification of principal axis, symmetry elements, definition and examples of molecules with different elements of symmetry including  $\sigma_v$ ,  $\sigma_h$ ,  $\sigma_d$

##### **2.2 Molecules with tri and tetracoordinate chiral centres:**

Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centres and their relative configurational stabilities.

##### **2.3 Molecules with two or more chiral centres:**

Configurational nomenclature, Constitutionally unsymmetrical molecules: Erythro-threo and syn-anti systems. Constitutionally symmetrical molecules with odd and even number of chiral centres: enantiomeric and meso forms, concept of stereogenic, chirotopic and pseudoasymmetric centres.

##### **2.4 Axial and Planar chirality:**

Principles of axial, planar and helical chirality, Stereochemical features and configurational descriptors (R,S) for the following classes of compounds: allenes, alkylidene



cycloalkanes, spiranes, biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes and helicenes.

### **2.5 Prochirality:**

Concept of prochirality, homotopic enantiotopic, and distereotopic ligand and faces: criteria based on symmetry and substitution/addition of molecules with different elements of chirality. Notation of prochirality, notation for molecules with pro-pseudo asymmetric centres. Notation for molecules with presence of a chiral and a pro-chiral centres. Top-right mnemonic.

## **Unit-III METHODS OF C-C BOND FORMATION USING THE CARBONYL FUNCTION [15L]**

**3.1** Reactivity of carbonyl group, Enols and enolates- Regioselective kinetic and thermodynamic enolate formation using LDA. Different types of aldol condensations under acid and base catalysis.

**3.2** Generation of dianion derived from active methylene compounds and regioselective C-C bond formation on unstabilized site.

**3.3** Mechanism, stereochemistry and applications of the following reactions: Acyloin, Benzoin, Claisen, Darzen, Dieckmann, Knoevenagel, Mannich, Michael, Robinson Annulation and Stobbe.

**3.4** Enamines as enolate equivalents. Metalloenamines, Synthesis of enamines and selected C-C bond formation.

## **Unit- IV SPECTROSCOPY [15L]**

### **4.1 UV-Visible Spectroscopy:**

Recapitulation of basic concepts and sample handling. Woodward-Fieser rules for calculation of  $\lambda_{\text{Max}}$  of conjugated dienes, polyenes, enones and aromatic carbonyl compounds.

Problems based on Woodward-Fieser rules.

### **4.2 IR Spectroscopy:**

Recapitulation of basic concepts and sample handling. Group frequencies and their use in detection and identification of functional groups.

### **4.3 PMR Spectroscopy:**

Recapitulation of basic concepts and sample handling. Prediction of structure of organic compounds based on the use of chemical shift and J values.

### **4.4 Mass Spectrometry:**

Recapitulation of basic concepts and sample handling. Fragmentation Pattern of major classes of organic compounds, Retro-Diels Alder reaction, McLafferty rearrangement and ortho effect.

**4.5** Structure determination of organic compounds involving individual or combined use of the above spectral techniques.

### **References Books:**

1. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A and B, Plenum Press.
3. Stereochemistry: Conformation and mechanism, P.S. Kalsi, New Age International, New Delhi.
4. Stereochemistry of carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Manden, Wiley.
5. Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri, New International Publishers Ltd.
6. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
7. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
8. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
9. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
10. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
11. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Nelson Thornes.
12. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
13. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks.
14. Spectrometric Identification of Organic Compounds, R. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley and Sons.
15. Organic Spectroscopy, William Kemp, W.H. Freeman & Company.
16. Organic Spectroscopy-Principles and Applications-Jagmohan, Narosa Publication.
17. Organic Spectroscopy, V.R. Dani, Tata McGraw Hill Publishing Co.
18. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Ltd.
19. Mechanism in Organic Chemistry, Peter sykes, 6<sup>th</sup> edition onwards.
20. Physical Organic Chemistry, Neil Isaacs
21. Modern Physical Organic Chemistry, Eric V. Anslyn and Dennis A. Dougherty

## IPCHEM 104: ANALYTICAL CHEMISTRY I

	<b>Unit I: Concepts of Analytical Chemistry</b>	<b>[15L]</b>
1.1	Concepts of Analytical Chemistry: Classification of Analytical Methods: An overview of Classical methods, Types of Instrumental methods	[2L]
	Selection of an analytical methods and their performance criteria.	[2L]
1.2	Concepts of optical methods: Electromagnetic spectrum, transitions, components in optical instruments, sources, description of LASER, wavelength selectors, monochromator functioning, effective band width, detectors and description of diode array type detector.	[6L]
1.3	Atomic Absorption Spectrometry: Principle, interferences, use of electro thermal analyser, hydride generator and cold vapour for trace metal analysis. Importance of electro thermal analyser for analysis of biological samples, level of detection; hydride generator for environmental samples and cold vapour technique for mercury analysis.	[5L]
	<b>Unit II: Atomic and molecular spectroscopy</b>	<b>[15L]</b>
2.1	Molecular transitions, derivative and dual wavelength spectroscopy. Application to trace analysis (d-d transition and charge transfer), biological samples and simultaneous determinations.	[5L]
2.2	Atomic Emission Spectroscopy based on plasma source, advantages of plasma source. Applications in geo-analysis, metal samples, agriculture and food samples and environmental analysis.	[5L]
2.3	Infrared spectroscopy: Concept of Fourier Transform Spectroscopy, instrumentation, advantages of FTIR and applications. Non-dispersive IR for detection of environmental gases.	[5L]
	<b>UNIT III: Separation methods</b>	<b>[15L]</b>
3.1	Solvent Extraction and Solid Phase Extraction: Recapitulation of basic concepts of solvent extraction and solid phase extraction. Liquid anion and cation exchangers. Mechanism of extraction. Extraction equilibria of metal chelates. Factors favoring solvent extraction of metal chelates. Sorbents.	[7L]
3.2	Chromatography: General classification of chromatographic methods. Concept of plate and rate theories: efficiency, resolution, selectivity and separation capability. Broadening of chromatographic peak and van Deemter equation. Optimization of chromatographic conditions.	[8L]
	<b>UNIT IV: Column chromatography techniques</b>	<b>[15L]</b>
4.1	Gas Chromatography: Principle of GLC and GSC; Instrumentation: carrier gas supply, sample introduction systems,	[4L]

packed & capillary columns; choice of detectors and comparative account of TCD, FID, ECD & thermionic detector. Temperature programming;

- 4.2 Applications in various fields. [3L]
- 4.3 High Performance Liquid Chromatography (HPLC): Types of liquid chromatography, column efficiency in LC; Instrument for LC: mobile phase reservoir and solvent treatment systems, pumping systems, sample introduction systems, columns, Detectors: UV, RI, EC and diode array. Modes of separation: partition, adsorption, ion exchange and size exclusion. [5L]
- 4.4 Applications in various fields. [3L]

#### Texts/ References:

1. D. A. Skoog, F. J. Holler, and T. A. Nieman, *Principles of Instrumental Analysis*, 5<sup>th</sup> ed., Philadelphia: Saunders College Publishing, 1998.
2. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 8<sup>th</sup> ed., Philadelphia: Saunders College Publishing, 2004.
3. G. D. Christian, *Analytical Chemistry*, 6<sup>th</sup> ed., John Wiley and Sons, New York, 2003.
4. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, *Vogel's Textbook of Quantitative Chemical Analysis*, 6<sup>th</sup> ed., ELBS, Longman Scientific & Technical, England, 2002.
5. H. H. Willard, L. L. Merrit, jr., J. A. Dean and F. A. Settle, Jr., *Instrumental Methods of Analysis*, 6<sup>th</sup> ed., CBS 1986.
6. R. D. Braun, *Introduction to Instrumental Analysis*, McGraw Hill, 1987.
7. G. H. Morrison and H. Freiser, *Solvent Extraction in Analytical Chemistry*, John Wiley & Sons, New York, 1966.
8. S. M. Khopkar, *Basic concept of Analytical Chemistry*, 3<sup>rd</sup> ed., Age International Publisher 2008.
9. T. Sekine and Y. Hasegawa, *Solvent Extraction chemistry*, Marcel Dekker, 1977.
10. P. G. Swell and B. Clarke, *Chromatographic Separations, Analytical Chemistry by open learning*, John Wiley & Sons, New York, 1987.
11. S. Sindsay, *High Performance Liquid Chromatography, Analytical Chemistry by open learning*, John Wiley & Sons, New York, 1987.
12. A. J. Bard and L. R. Faulkner, *Electrochemical Methods*, Wiley, New York, 1980
13. A. M. Bond, *Modern Polarographic Methods in Analytical Chemistry*, Marcel Dekker, New York, 1980.
14. L. C. Thomas and G. J. Chamberline, *Colorimetric Analytical Methods*, 9<sup>th</sup> ed., The Fintometer Ltd., Salisbury, England, 1980.
15. T. C. Morrili, R. m. Silverstein and G. C. Bassler, *Spectrometric Identification of Organic Compounds*, Wiley, 1981.
16. Vogel's Text Book of Quantitative Organic Analysis, 2<sup>th</sup> ed. ELBS.
17. R. A. Day, Jr. and A. L. Underwood, *Quantitative Analysis*, 6<sup>th</sup> ed., Prentice Hall of India Pvt. Ltd., New Delhi, 1993.
18. Jared L. Anderson, Alain Berthod, Veronica Pino, and Apryll M. Stalcup (ed), *Analytical Separation Science (Volume 1-5)*. WILEY-VCH 2015.
19. Jack Cazes (ed) *Ewing's Analytical Instrumentation Handbook*, 3<sup>rd</sup> edition, Marcel Dekker 2009.
20. R. Kellner, J.M. Mermet, M. Oto, M. Valcarcel, H. M. Widmer (ed), *Analytical Chemistry: A modern Approach to Analytical Science 2<sup>nd</sup> edition*. WILEY-VCH 2004.

21. Solid phase Extraction- Principles, Techniques and Applications, N. J. K. Simpson, Marcel Dekker, New York, (2000).

### **IPCHEM 105: PHYSICAL CHEMISTRY PRACTICAL-I**

#### **Instrumental Experiments:**

##### ***Conductometry and Potentiometry***

1. Titration of a mixture of trichloroacetic acid, monochloroacetic acid and acetic acid with sodium hydroxide conductometrically.
2. Verification of Ostwald's dilution law and determination of the dissociation constant of a weak monobasic acid conductometrically.
3. Study of the effect of substituent on dissociation constant of acetic acid conductometrically.
4. Determination of concentrations and amounts of iodide, bromide and chloride in the mixture by potentiometric titration with silver nitrate.
5. Determination of solubility product of silver chloride potentiometrically using a concentration cell.
6. Determination of the formula of the silver-ammonia complex by potentiometric method.
7. Determination of  $pK$  values of phosphoric acid by potentiometric titration with sodium hydroxide using a glass electrode.
8. Determination of acidic and basic dissociation constants of an amino acid and hence the isoelectric point of the acid.

### **IPCHEM-106: INORGANIC CHEMISTRY PRACTICAL-I**

#### **Synthesis, Purification and Analysis of the following Inorganic Preparations:**

1. Potassium trioxalatochromate (III)
2. Bis(ethylenediamine) copper (II) sulphate
3. Hexamine nickel (II) chloride/sulphate
4. Potassium dioxalatochromate(II) dihydrate
5. Potassium trioxalatoaluminum(III) hydrate

#### **Reference books:**

1. A. I. Vogel, Vogel's Text Book of Quantitative Inorganic Analysis, 6<sup>th</sup> Ed., Pearson Education, 2000.
2. J. D. Woolins, Inorganic Experiments, Wiley-VCH Verlag GmbH and Co., 2003.
3. W. G. Palmer, Experiments in Inorganic Chemistry, Cambridge University Press, 1954.
4. G. Raj, Advanced Practical Inorganic Chemistry,
5. G. Brauer, Handbook of Preparative Inorganic Chemistry, Vol. 1 and 2, Academic Press, 1967.

6. G. Marr and B. W. Rockette, Practical Inorganic Chemistry, Van NostrnadReinhond, 1972.
7. G. Pass and H. Sutcliffe, Practical Inorganic Chemistry, 2<sup>nd</sup> Ed., Chapman and Hall, 1985.

### **IPCHEM 107: ORGANIC CHEMISTRY PRACTICAL-I**

#### **One step preparations (0.5 to 1.0 g scale):**

The candidate is expected to perform any 10 of the following preparations and submit the crystallized preparation and TLC analysis of the purified product, mp, % yields, etc.

1. Bromobenzene to p-nitro bromobenzene
2. Nitrobenzene to m-dinitrobromobenzene
3. Benzoin to Benzil
4. Anthracene to Anthraquinone
5. o-phenylenediamine to 2-methyl benzimidazole
6. o-phenylenediamine to 2,3-diphenylquinoxaline
7. Anthracene-Maleic Anhydride adduct
8. p-bromoacetanilide to p-bromoaniline
9. 5,5-diphenylhydantoin from urea and benzil
10. p-benzoquinone to 1,2,4-triacetoxybenzene
11. 2-naphthol to BINOL
12. o-phenylenediamine to benzotriazole

#### **Reference Books:**

1. Elementary Practical Organic chemistry Part-I small scale preparations, A.L. Vogel (Longman)
2. Laboratory Manual of organic chemistry, B.B. Dey and M.V. Sitaram revised by T.R Govindachari (Allied Publishers Ltd. )

### **IPCHEM 108: ANALYTICAL CHEMISTRY PRACTICAL-I**

#### ***Non-Instrumental Experiments:***

1. Calibration of a 10 mL pipette by weighing at room temperature and reporting the result with statistical data.
2. Determination of Manganese from pyrolusite by potassium permanganate method.
3. Estimation of vitamin C by titration with potassium bromate.

4. Determination of number of nitro group in organic compound by titanium method.
5. Separation and determination of Fe (III) and Mg (II) /Zn (II) using ethyl acetate /ether as a solvent.
6. Determination of the exchange capacity of a cation ion exchange resin

### SEMESTER-II

Course Code	Title of the Course	No. of Credits	No. of hours per SEMESTER-R	Examination		Total Marks
				Mid Sem Marks	End-Sem Marks	
IPCHEM 201	Physical Chemistry II	4	60	40	60	100
IPCHEM 202	Inorganic Chemistry II	4	60	40	60	100
IPCHEM 203	Organic Chemistry II	4	60	40	60	100
IPCHEM 204	Analytical Chemistry II	4	60	40	60	100
IPCHEM 205	Physical Chemistry Practical II	2	-	-	50	50
IPCHEM 206	Inorganic Chemistry Practical II	2	-	-	50	50
IPCHEM 207	Organic Chemistry Practical II	2	-	-	50	50
IPCHEM 208	Analytical Chemistry Practical II	2	-	-	50	50
	Total	24			Total	600

**\*Practical component involves 16 h per week laboratory work for 15 weeks.**



## **SYLLABUS: SEMESTER-II**

### **IPCHEM 201: PHYSICAL CHEMISTRY-II**

#### **Unit-I THERMODYNAMICS-II [15 L]**

Partial molar quantities, chemical potential for ideal gas, gas mixtures, Gibbs free energy of mixing, entropy and volume of mixing, Gibbs Duhem equation, Variation of chemical potential with pressure and temperature.

Excess functions (Chemical potential, Gibbs free energy and enthalpy function), Equilibrium constant and its dependence on temperature and pressure.

#### **Unit-II APPLIED ASPECTS OF QUANTUM CHEMISTRY**

[15L]

##### **Application of Quantum Chemistry in Vibrational motion:**

The one-dimensional harmonic oscillator: Classical and Quantum mechanical treatment, Hermite polynomials, Wavefunctions, probability densities, and energy levels

##### **Application of Quantum Chemistry in Rotational motion:**

Spherical polar coordinates, Separation of variables, The rigid rotor: Legendre functions, energy levels and wave functions\*.

##### **Application of Quantum Chemistry in Atomic system:**

The hydrogen atom and hydrogen-like ions, Reduction of the two-particle problem to two one-particle problems, Solutions to  $R(r)$ ,  $\Theta(\theta)$  and  $\Phi(\phi)$  equations\*, Hydrogen-like orbitals, sketches of wave functions ( $\psi$ ) and probability densities ( $|\psi|^2$ ), polar plots of angular parts, orbital and spin angular momentum, spin orbitals.

#### **Unit-III APPLICATIONS OF THERMODYNAMICS AND ELECTROCHEMISTRY [15L]**

Experimental techniques for determination of thermodynamic quantities: Bomb Calorimeter, Coffee Cup Calorimeter, Differential Scanning Calorimeter.

Exergonic and endergonic reactions, Thermodynamics of ATP, applications of thermodynamics to ultra-purity and controlled purity (Zone Refining and zone levelling).

Debye-Hückel theory of strong electrolyte, ionic atmosphere, activity coefficients of electrolyte solutions- Debye-Hückel limiting law, extension to higher concentrations.

Electrolytic conductance and ion-ion interactions, Debye-Hückel-Onsager equation, validity of equation, Debye-Falkenhagen effect, Wien effect, weak electrolyte and Debye-Huckel theory.

Determination of thermodynamic functions of cell reaction.

Electrochemistry in water and effluent treatment.



### **Unit-IV MOLECULAR REACTION DYNAMICS [15L]**

Collision theory, steric factor, activated complex theory, reaction coordinate and transition state, thermodynamic aspects, reaction between ions, salt effects, dynamics of molecular collisions.

Homogeneous catalysis – enzyme catalysis, Michaelis-Menten mechanism, acid base catalysis.

Heterogeneous catalysis – Examples: hydrogenation, oxidation, cracking and forming.

***\*Derivation not expected***

***Note: Numerical and theoretical problems from each Unit- are expected.***

#### **Reference books:**

1. Peter Atkins and Julio de Paula, *Atkin's Physical Chemistry*, 7<sup>th</sup> ed., Oxford University Press, 2002.
2. K. J. Laidler and J. H. Meiser, *Physical Chemistry*, 2<sup>nd</sup> ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3<sup>rd</sup> ed., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5<sup>th</sup> ed., Tata McGraw-Hill, New Delhi, 2002.
5. G. W. Castellan, *Physical Chemistry*, 3<sup>rd</sup> ed., Narosa Publishing House, New Delhi, 1983.
6. D. A. McQuarrie and J. D. Simon, *Physical Chemistry - a molecular approach*, Viva Books Private Limited, New Delhi, 1998.
7. S. Glasstone, *Text Book of Physical Chemistry*, 2<sup>nd</sup> ed., McMillan and Co. Ltd., London, 1962.
8. Derek Pletcher, *Industrial Electrochemistry*, London New York.
9. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
10. Ira N. Levine, *Quantum Chemistry*, 5<sup>th</sup> ed., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
11. J. P. Lowe, *Quantum Chemistry*, 2<sup>nd</sup> ed., Academic Press, New York, 1993.
12. R. Anantharaman, *Fundamentals of Quantum Chemistry*, McMillan India Limited, 2001.
13. Mahendra R. Awode, *Quantum Chemistry*, S. Chand and Co. Ltd., New Delhi, 2002.
14. R. K. Prasad, *Quantum Chemistry*, 2<sup>nd</sup> ed., New Age International Publishers, 2000.
15. D. O. Hayward, *Quantum Mechanics for Chemists*, Royal Society for Chemists, 2002.
16. Samuel Glasstone, *An introduction to electrochemistry*, East West edition, New Delhi.
17. G. L. Agarwal, *Basics Chemical kinetics*, Tata McGraw Hill, New Delhi.
18. D. R. Crow, *Principles and Applications of Electrochemistry*, 4<sup>th</sup> edition, Blackie, London, 1994.

19. J.O'm. Bockris and A. K. N. Reddy, *Modern Electrochemistry*-Vol. 1 and 2, Plenum press, New York.
20. R. A. Robinson and R.H. Stokes, *Electrolyte Solutions*, 2<sup>nd</sup> Edition, Butterworths, London 1959.
21. R. P. Rastogi, R. R. Mishra, *An Introduction to Chemical Thermodynamics*, Vikas Publishing House Pvt. Ltd.
22. K. J. Laidler, *Chemical Kinetics*, 3<sup>rd</sup> ed., Pearson Education.

**List of Books for further reading:**

1. W. G. Davis, *Introduction to Chemical Thermodynamics – A Non-Calculus Approach*, Saunders, Philadelphia, 1972.
2. I. M. Klotz and R. M. Rosenberg, *Chemical Thermodynamics*, 5<sup>th</sup> ed., John Wiley and Sons, Inc., 1994.
3. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.

**IPCHEM-202: INORGANIC CHEMISTRY-II**

**Unit-I**      **SOLID STATE CHEMISTRY AND NANOMATERIALS**      **[15L]**

**(A) Solid State Chemistry**

- (i) Recapitulation of basic solid state chemistry.
- (ii) Structures of compounds of the type: AB [zinc sulfide (ZnS), nickel arsenide (NiAs)], AB<sub>2</sub> [fluorite (CaF<sub>2</sub>), antiferite (Na<sub>2</sub>O), rutile (TiO<sub>2</sub>) and layer structures viz., cadmium chloride (CdCl<sub>2</sub>) and cadmium iodide, (CdI<sub>2</sub>)].
- (iii) Principles, merits and demerits with suitable examples of: ceramic method, precursor method, sol-gel method, microwave synthesis for the preparation of inorganic solids.

**(B) Nanomaterials**

- (i) Introduction to nanomaterials.
- (ii) **Preparative methods:** Chemical methods, Biological methods; Role of capping agents.
- (iii) Applications of nanomaterials in electronics and biomedical field.

**Unit-II**      **MOLECULAR SYMMETRY AND GROUP THEORY**      **[15L]**

- (i) Symmetry elements and symmetry operations, product of symmetry operations, Cartesian coordinate system and symmetry elements.
- (ii) Symmetry classification of molecules: point groups, mathematical requirement for a point group, systematic assignment of point groups to molecules.
- (iii) Identification of molecular point groups of molecules having low

symmetry, high symmetry and special symmetry.

- (iv) Descent in symmetry of molecules with substitution.
- (v) Group multiplication tables, classes of symmetry operations.
- (vi) Symmetry criteria for optical activity, Symmetry restrictions on dipole moment.

**Unit-III ENVIRONMENTAL CHEMISTRY**

**[15L]**

**(i) Chemical Toxicology:**

toxic chemicals in the environment, biochemical effects and speciation of toxic elements like arsenic, lead, mercury and cadmium; antidotes for the toxic elements. Biochemical effects of fluoride and pesticides.

**(ii) Radiation pollution:**

Sources and biological implication of radioactive pollutants.

**(iii) Solar energy:**

Use of solar energy in space heating and water heating; Production of electricity using solar trough collectors, Power tower and solar pond; solar energy for driving vehicles.

**(iv) Power from other sources:**

Hydro power, Wind power, Geothermal energy, Ocean thermal energy conversion (OTEC), Tidal power.

#### **Unit-IV    BIOINORGANIC CHEMISTRY**

[15L]

(i) **Biological oxygen carriers:**

Myoglobin, hemoglobin, hemerythrene and hemocyanine. Biochemical effect of cyanide, Hill equation, Bohr effect and their implications.

(ii) Reactions of dioxygen in biological system with examples of peroxidase, monooxygenase, superoxide dismutase and oxidase reactions.

(iii) **Nitrogen fixation:** Nitrogenase, Hydrogenases.

(iv) **Metal ion transport and storage:** Ionophores, transferrin and Ferritin.

(v) **Metal ions in medicines:** cis-platin and related compounds.

#### **Reference books:**

##### **Unit-I**

1. A. R. West, Solid State Chemistry and Its Applications, John Wiley & Sons, 1987.
2. L. V. Azaroff, Introduction to solids, Tata McGraw Hill Book Co, 1977.
3. H. V. Keer, Principles of Solid State, Wiley Eastern Ltd., 1993.
4. C. N. R. Rao and G. Gopalkrishnan, New Directions in solid state chemistry, 2<sup>nd</sup> Ed., Cambridge University Press, 1997.
5. Lesley E. Smart and Elaine A. Moore, Solid State Chemistry – An introduction, 3<sup>rd</sup> Ed., Taylor and Francis, 2005.
6. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone, 2014.
7. S. K. Kulkarni, Nanotechnology-Principles and Practices, Capital Publishing Co., 2007.
8. G. Cao, Nanostructures and Nanomaterials- Synthesis, Properties and Applications, Imperial college Press, 2004.
9. C. N. R. Rao, A. Muller and A. K. Cheetham, The Chemistry of Nanomaterials- Synthesis, Properties and Applications, Volume-I, Wiley VCH, 2004.

##### **Unit-II**

1. K.V.Reddy, Symmetry and Spectroscopy of Molecules, 2<sup>nd</sup> Ed., New Age International Publishers 2009.
2. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, 1998.
3. A.S. Kunju and G. Krishnan, Group Theory and its Applications in Chemistry, PHI-Learning, 2010.
4. F. A. Cotton, Chemical Applications of Group Theory, 2<sup>nd</sup> Ed., Wiley Eastern Ltd., 1989.
5. G. Raj, A. Bhagi and V. Jain, Group Theory and Symmetry in Chemistry, 3<sup>rd</sup> Ed., Krishna Prakashan, 2010.
6. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5<sup>th</sup> Ed., Oxford University Press, 2010.

7. R. S. Drago, Physical Methods in Inorganic Chemistry, Affiliated East-West Press Pvt. Ltd., 2014.

### **Unit-III**

1. A. K. De, Environmental Chemistry, 7<sup>th</sup> Ed., New Age International Publishers, 2007.
2. G. S. Sodhi, Fundamental Concepts of Environmental Chemistry, 3<sup>rd</sup> Ed., Narosa Publishing House, 2013.
3. S. S. Dara and D. D. Mishra, A Textbook of Environmental Chemistry and Pollution Control, S. Chand & Company Ltd., 2012.
4. D. Banerjea, Coordination Chemistry, Tata Mc Graw Hill, 1993.
5. S. K. Banerji, Environmental Chemistry, 2<sup>nd</sup> Ed., Prentice-Hall of India, 2005.
6. R. A. Bailey, H. M. Clark, J. P. Ferris, S. Krause and R. L. Strong, Chemistry of Environment, 2<sup>nd</sup> Ed., Academic Press, 2005.
7. J. E. Girard, Principles of Environmental Chemistry, 2<sup>nd</sup> Ed., Jones and Bartlett publishers, 2011.
8. H. Kaur, Environmental Chemistry, Pragati Prakashan, 8<sup>th</sup> Ed., 2014.

### **Unit-IV**

1. I. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, Bioinorganic Chemistry, 1<sup>st</sup> Indian Ed., Viva Books, 1998.
2. D. Banerjea, Coordination Chemistry, Tata Mc Graw Hill, 1993.
3. R. W. Hay, Bioinorganic Chemistry, Ellis Harwood, 1984.
4. J. A. Cowan, Inorganic Biochemistry-An introduction, VCH Publication, 1993.
5. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Publications, Mill Valley, Caligrionic, 1994.
6. G. N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, Dhuri& Sons, 1988.

## **IPCHEM 203: ORGANIC CHEMISTRY-II**

### **Unit-IPHYSICAL ORGANIC CHEMISTRY AND AROMATICITY [15L]**

- 1.1 Transition state theory, Arrhenius equation and its application to estimate  $E_{act}$ , Hammond's postulate, Principle of microscopic reversibility, Kinetics  $v \propto$  Thermodynamic control.
- 1.2 Influence of solvent polarity, solvent scales (Y-scale), solvatochromism, (Z and ET Scales), ionic strengths and salt effect, Acid-base catalysis, Bronsted catalysis equation.
- 1.3 Structural, thermochemical and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems, DRE and REPE, London Diamagnetism, Diamagnetic exaltation and concept of closed configuration.
- 1.4 Application of HMO theory to monocyclic conjugated systems, Frost-Musulin diagrams, Huckel's  $(4n+2)$   $\pi$  electron rule, Exceptions to  $(4n+2)$   $\pi$  electron rule and  $4n$  rules.

**1.5** Aromatic, Antiaromatic and Homoaromatic compounds upto 18 carbon atoms. Aromaticity of benzenoid systems, heterocycles, metallocenes, azulenes, annulenesconjugated molecules with exocyclic double bonds and tropylium cations.

## **Unit-II ELIMINATION AND NUCLEOPHILIC SUBSTITUTION REACTIONS**

[15 L]

- 2.1 Types of elimination reactions, E<sub>1</sub> and E<sub>2</sub> mechanisms.
- 2.2 Orientation of elimination reactions: Saytzeff and Hoffmann rules. E<sub>2</sub> reactions of vinyl halide, E<sub>1cB</sub> mechanism.
- 2.3 Pyrolytic elimination: Chugaev reaction, Cope reaction, Hoffmann's and Pyrolysis of acetates.
- 2.4 Aliphatic nucleophilic substitution at sp<sup>3</sup> carbon: S<sub>N</sub><sup>1</sup>, S<sub>N</sub><sup>2</sup>, S<sub>N</sub><sup>i</sup>, S<sub>N</sub>cA reactions. Ion pair in S<sub>N</sub><sup>1</sup> reactions, Stereochemistry of all the above reactions, Factors affecting these reactions: substrate nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group.
- 2.5 Nucleophilic substitution reactions at sp<sup>2</sup> (vinylic) carbon.
- 2.6 Aromatic nucleophilic substitution reaction: S<sub>N</sub>Ar, S<sub>N</sub><sup>1</sup>, Benzyne mechanism, ipso, cine and tele substitutions, vicarious substitution.

## **Unit-III OXIDATION-REDUCTION [15 L]**

### **3.1 Preparation of reagents (wherever applicable), mechanism and applications of the following:**

Epoxidation, Baeyer-Villiger Oxidation and Oppenauer Oxidation. Oxidations using Osmium Tetroxide, Lead Tetraacetate, Periodic acid, Selenium dioxide, PCC and PDC.

### **3.2 Dehydrogenation with DDQ and TCQ, and Ozonolysis**

### **3.3 Preparation of reagents (wherever applicable), mechanism and applications of the following:**

Wolf-Kishner reduction, Clemmensen reduction, Meerwein-Ponndorf-Verley reduction, Birch reduction, Reductions with NaBH<sub>4</sub>, LiAlH<sub>4</sub> and DIBAL.

### **3.4 Homogeneous reductions: Wilkinson's catalysts and related systems.**

## **Unit-IV REACTIONS AND REARRANGEMENTS [15 L]**

### **4.1 Mechanism, stereochemistry (if applicable) and applications of the following:**

Arndt-Eistert reaction, Baylis-Hilman reaction, McMurry Coupling, Mitsunobu reaction and Mukiyama esterification, Woodward Prevost Hydroxylation.

### **4.2 Mechanism, stereochemistry (if applicable) and applications of the following:**

Cope rearrangement, Claisen rearrangement, Dienone-Phenol rearrangement, Favroskii rearrangement, Fries rearrangement and Tiffeneau-Demjanov rearrangement.

### **4.3 Ester hydrolysis (all 8 mechanisms of acid and base catalyzed hydrolysis)**

### **Reference books:**

1. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A, page no. 713-769, and B, Plenum Press.



3. Stereochemistry: Conformation and mechanism, P.S. Kalsi, New Age International, New Delhi.
4. Stereochemistry of carbon compounds, E.L Eliel, S.H Wilen and L.N Manden, Wiley.
5. Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri. New International Publishers Ltd.
6. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
7. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
8. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
9. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
10. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
11. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.
12. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
13. Mechanism in Organic Chemistry, Peter sykes, 6<sup>th</sup> edition onwards.
14. Physical Organic Chemistry, Neil Isaacs
15. Modern Physical Organic Chemistry, Eric V. Anslyn and Dennis A. Dougherty
16. Comprehensive Organic chemistry, Barton and Ollis, Vol 1, Page No. 215-240.

### **IPCHEM 204: ANALYTICAL CHEMISTRY-II**

#### **Unit-I: ELECTROANALYTICAL CHEMISTRY [15L]**

##### **1.1 Ion selective potentiometry:**

Basic concept, solid state, precipitate and liquid-liquid membrane, enzyme and gas sensing electrodes with applications. [8L]

##### **1.2 Introduction to modern voltammetric techniques:**

Differential pulse polarography, Cyclic voltammetry and Stripping (cathodic & anodic) voltammetry. [7L]

#### **Unit-II: SPECTROSCOPIC METHODS [15L]**

##### **2.1 Magnetic resonance spectroscopy:**

Basic principles, instrumentation and sample handling, Quantitative applications of proton NMR, Introduction to Carbon-13, Phosphorous-31 and Fluorine-19 with applications. [8L]

##### **2.1 Mass spectrometry:**

Recapitulation, instrumentation; ion sources for molecular studies; electron impact, chemical ionization field ionization, field desorption, fast atom bombardment and MALDI sources. Mass analyzers: quadrupole, time of flight and ion trap, applications. [7L]

### **Unit-III: MISCELLANEOUS TECHNIQUES [15L]**

#### **3.1 X-ray spectroscopy:**

Principles, instrument components and applications of X-ray fluorescence, absorption and diffraction methods. [8L]

#### **3.2 Introduction to surface analytical techniques. [3L]**

#### **3.3 Electron Spectroscopy for Chemical Analysis: Principle, Instrumentation and applications. [4L]**

### **Unit-IV: AUTOMATION IN CHEMICAL ANALYSIS AND ELECTROPHORESIS [15L]**

#### **4.1 An overview of automated instruments and instrumentation, process control analysis; Types of automatic analytical systems: Flow injection analysis, automatic organic elemental analyzers, Gas monitoring equipment. [8L]**

#### **4.2 Electrophoretic methods [7L]**

### **Reference books:**

1. D. A. Skoog, F. J. Holler, and T. A. Nieman, *Principles of Instrumental Analysis*, 5<sup>th</sup> ed., Philadelphia: Saunders College Publishing, 1998.
2. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 8<sup>th</sup> ed., Philadelphia: Saunders College Publishing, 2004.
3. G. D. Christian, *Analytical Chemistry*, 6<sup>th</sup> ed., John Wiley and Sons, New York, 2003.
4. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, *Vogel's Textbook of Quantitative Chemical Analysis*, 6<sup>th</sup> ed., ELBS, Longman Scientific & Technical, England, 2002.
5. H. H. Willard, L. L. Merritt, jr., J. A. Dean and F. A. Settle, Jr., *Instrumental Methods of Analysis*, 6<sup>th</sup> ed., CBS 1986.
6. R. D. Braun, *Introduction to Instrumental Analysis*, McGraw Hill, 1987.
7. G. H. Morrison and H. Freiser, *Solvent Extraction in Analytical Chemistry*, John Wiley & Sons, New York, 1966.
8. S. M. Khopkar, *Basic concept of Analytical Chemistry*, 3<sup>rd</sup> ed., Age International Publisher 2008.
9. T. Sekine and Y. Hasegawa, *Solvent Extraction chemistry*, Marcel Dekker, 1977.
10. P. G. Swell and B. Clarke, *Chromatographic Separations, Analytical Chemistry by open learning*, John Wiley & Sons, New York, 1987.
11. S. Sindsay, *High Performance Liquid Chromatography, Analytical Chemistry by open learning*, John Wiley & Sons, New York, 1987.
12. A. J. Bard and L. R. Faulkner, *Electrochemical Methods*, Wiley, New York, 1980
13. A. M. Bond, *Modern Polarographic Methods in Analytical Chemistry*, Marcel Dekker, New York, 1980.
14. L. C. Thomas and G. J. Chamberline, *Colorimetric Analytical Methods*, 9<sup>th</sup> ed., The Fintometer Ltd., Salisbury, England, 1980.

15. T. C. Morrili, R. m. Silverstein and G. C. Bassler, *Spectrometric Identification of Organic Compounds*, Wiley, 1981.
16. Vogel's Text Book of Quantitative Organic Analysis, 2<sup>th</sup> ed. ELBS.
17. R. A. Day, Jr. and A. L. Underwood, *Quantitative Analysis*, 6<sup>th</sup> ed., Prentice Hall of India Pvt. Ltd., New Delhi, 1993.
18. Jared L. Anderson, Alain Berthod, Veronica Pino, and Apryll M. Stalcup (ed), *Analytical Separation Science (Volume 1-5)*. WILEY-VCH 2015.
19. Jack Cazes (ed) *Ewing's Analytical Instrumentation Handbook*, 3<sup>rd</sup> edition, Marcel Dekker 2009.
20. R. Kellner, J.M. Mermet, M. Oto, M. Valcarcel, H. M. Widmer (ed), *Analytical Chemistry: A modern Approach to Analytical Science 2<sup>nd</sup> edition*. WILEY-VCH 2004.

## **IPCHEM 205: PHYSICAL CHEMISTRY PRACTICAL-II**

### **Non-Instrumental Experiments:**

#### ***Thermodynamics, Phase Rule and Reaction Kinetics:***

1. Determination of heat of solution of benzoic acid by solubility measurements.
2. Determination of heat of solution of salicylic acid by solubility measurements.
3. Study of three-component system: Water-Acetic acid-Chloroform.
4. Study of three-component system: Water-Toluene-Acetic acid.
5. Study of variation of solubility of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product. (Complexometric titration with EDTA)
6. Determination of equilibrium constant of the reaction  $KI + I_2 \rightleftharpoons KI_3$  by distribution method.
7. Investigation of the reaction between acetone and iodine.

## **IPCHEM-206: INORGANIC CHEMISTRY PRACTICAL-II**

### **Analysis of Complex Materials:**

1. Devarda's Alloy: Cu by EDTA method, Al by Gravimetry using oxine
2. Cu-Ni Alloy: Cu by iodometric method; Ni gravimetrically by DMG method.
3. Solder Alloy: Sn gravimetrically by oxide method; Pb by EDTA method.
4. Lime Stone Ore: Loss on ignition; Ca by EDTA method.
5. Haematite Ore: Acid insoluble residue; Fe by redox titration.

### **Reference books:**

1. A. I. Vogel, Vogel's Text Book of Quantitative Inorganic Analysis, 6<sup>th</sup> Ed., Pearson Education, 2000.
2. J. D. Woolins, Inorganic Experiments, Wiley-VCH Verlag GmbH and Co., 2003.
3. W. G. Palmer, Experiments in Inorganic Chemistry, Cambridge University Press, 1954.
4. G. Raj, Advanced Practical Inorganic Chemistry,
5. G. Brauer, Handbook of Preparative Inorganic Chemistry, Vol. 1 and 2, Academic Press, 1967.
6. G. Marr and B. W. Rockette, Practical Inorganic Chemistry, Van Nostrand Reinhold, 1972.
7. G. Pass and H. Sutcliffe, Practical Inorganic Chemistry, 2<sup>nd</sup> Ed., Chapman and Hall, 1985.

## **IPCHEM 207: ORGANIC CHEMISTRY PRACTICAL-II**

### **Separation of Binary mixture by microanalytical technique**

Separation of binary mixture using physical and chemical methods. Identification of one of the compounds and checking its purity by TLC. Preparation of the derivative of one of the compounds. The following types are expected: (i) Solid-Solid (ii) Non-volatile liquid-Non-volatile liquid (iii) Water-soluble/insoluble solid-Non-volatile liquid with compounds from the same or different chemical classes in all three categories.

The candidate is expected to carry out separation of 10 mixtures.

### **Reference Books:**

1. Systematic Qualitative organic analysis, H. Middleton (Orient Longman)
2. A Handbook of Organic Analysis, H.T. Clark (Orient Longman)
3. Systematic Identification of organic compounds, R.L. Shriner (John Wiley, New York)

### **IPCHEM 208: ANALYTICAL CHEMISTRY PRACTICAL-II**

#### **Instrumental Experiments:**

1. Non aqueous titration: Determination of sodium benzoate / glycine by using perchloric acid in glacial acetic acid by potentiometry using glass-calomel system.
2. Determination of glucose by Folin-Wu method.
3. Determination of nitrite in a water sample by colorimetric method.
4. Determination of chromium and manganese by simultaneous spectrophotometry.
5. Determination of silica by Molybdenum Blue method.
6. Flame Photometric determination of Li /Na/K by standard addition method.

**SEMESTER-III**

Course Code	Title of Course	No. of Credits	No. of Hours	Examination		Total Marks
				Continuous Evaluation	End SEM	
IPCHEM 351	Basics of Polymer, Rubber & Additives	04	60	40	60	100
IPCHEM 352	Rheology & Processing Rubbers	04	60	40	60	100
IPCHEM 353	Testing of Rubber, allied materials & composites	04	60	40	60	100
IPCHEM 354 EC-I	Biopolymers and Bio composites	04	60	40	60	100
IPCHEM 355 EC-II	Polymer Nano Composites	04	60	40	60	100
IPCHEM 356	Industrial Polymer Chemistry Practical-I	04	-	-	100	100
IPCHEM 357	Industrial Polymer Chemistry Practical-II	04	-	-	100	100

**No. of CREDITS: 24**

**TOTAL MARKS: 600**

**Note: Students will have to select one of the electives i.e. IPCHEM 354 EC-I or  
IPCHEM 355 EC-II**

**Practical component involves 16 hour per week of laboratory work for 15 weeks**

## SYLLABUS: SEMESTER III

### IPCHEM 351: BASICS OF POLYMERS, RUBBER AND ADDITIVES

#### Unit I POLYMERS & POLYMERIZATION TECHNIQUES

[15L]

**Polymers:** monomer, oligomer and polymer, Average Molecular Weight, Molecular weight, Distribution & Poly dispersity Index, classification of polymers, structure of polymer. Types of polymerization.

**Polymerization Techniques:** Mass Polymerization, Bulk Polymerization, Solution Polymerization, Emulsion Polymerization, Suspension Polymerization, Mechanisms with explanation. Characteristics, Relative advantages and disadvantages.

**Classification of Polymers:** Natural and synthetic polymers, Biopolymers, thermoplastic, thermosets, Elastomers, Fibers etc.

**Structure Property Relationship in Polymers:** Structure of polymers, amorphous, semi-crystalline and crystalline states in polymers, glass transition, melting and crystallization temperature. Effect of structure on the chemical, mechanical, electrical and optical properties of polymers.

#### Unit II GENERAL PURPOSE RUBBER

[15L]

**Natural Rubber (NR):** Origin–Natural Rubber Latex, tapping, processing, properties and applications – Conversion of Latex into dry rubber – Properties of dry rubber – Classification based on technical specifications – Modifications of Natural Rubber

**Styrene-Butadiene Rubber (SBR):** Introduction, polymerization, types of SBR, structure & property variation in Emulsion SBRs and Solution SBRs. Compounding, Processing, Applications.

**Polybutadiene Rubber (PBR):** Manufacture, Structure and Properties of Polybutadienes, Processing and Applications.

**Synthetic Polyisoprene (IR) Rubbers:** Preparation of Synthetic Polyisoprene (IR) Rubbers, Properties, IISRP Numbering System, Processing, Applications.

#### Unit III SPECIAL PURPOSE RUBBER

[15L]

**Preparation, properties and Application of:** Nitrile Rubber & modified NBR (HNBR & XNBR), Butyl Rubber & Halogenated butyl rubbers, Polychloroprene Rubbers, Ethylene Propylene Rubber and Ethylene Vinyl acetate copolymers – Elastomers based on modified polyethylene (chlorinated polyethylene & chlorosulphonated polyethylene), Acrylate rubbers, Polysulphide rubbers, Hydrin rubbers, Silicones and Fluoroelastomers etc.

**Rubber blends:** miscible and immiscible blends,

**Thermoplastic Elastomers – Preparation, properties and Application of:** SBS and SIS Block copolymers, Thermoplastic Polyurethane elastomers, Thermoplastic-co-polyesters, Thermoplastic elastomers based on Plastics, Dynamic Vulcanization

#### Unit IV NON-RUBBER ADDITIVES

[15L]

**Part A: Vulcanizing ingredients & other additives:** Vulcanizing ingredients & their sequence of mixing: Activators and Accelerators: mechanisms of action. Other

cure systems based on metal oxides, peroxides, etc. retarders, inhibitors anti-reversion agents.

#### **Part B: Fillers**

**Carbon black**-Its preparation, structure, properties and their effect on rubber properties

**Silica** fillers & coupling agents, Other fillers: Clay, Calcium carbonate, titania etc. Nano-fillers:

**Reinforcement by filler:** Reinforcement, Factors influencing elastomers reinforcement, fillers characteristics, main effects of fillers on vulcanizate properties, Influence of fillers characteristics on the cross linking process, Filler incorporation, the role of bound rubber, reinforcement and crosslink density.

**Part C: Processing aids & other additives:** Processing aids, plasticizers, process additives, release agents, Other additives like colourants, blowing agents, factice, Fire Retardants, Antistatic Agents, Deodorants and Reodorants, Biocides and Fungicides etc. **Antidegradants:** Introduction, Autoxidation of Hydrocarbon Polymers, Amine & Phenolic Antioxidants & other types, Antizonants, Prevention of Ozone Attack with the use of waxes & saturated polymer for Ozone Protection.

#### **References:**

1. F. W. Billmeyer Jr., Text Book of Polymer Science, Ed. Wiley-Interscience, 1984.
2. V. T. Gowariker, N. V. Viswanathan, and J. Sreedar, Polymer Science, 1988.
3. M. Morton, Rubber Technology, Chapman Hall, 1995.
4. J. Brydson, Rubber Chemistry, Butterworths, 1978
5. B. Kothandaraman, Rubber Materials, Ane Books, 2008.
6. I. Franta, Elastomers and Rubber Compounding materials, Elsevier, 1989.
7. B. Kothandaraman, Rubber Materials, Ane Books, 2008.

### **IPCHEM 352: RHEOLOGY AND PROCESSING OF RUBBERS**

#### **Unit I RHEOLOGY OF RUBBERS**

[12L]

Definition of Rheology, Rheological Perspective, The importance of nonlinearity, Solids and liquids, Components of rheological research: Rheometer, Constitutive equations, Complex flows of elastic liquids.

#### **Unit II COMPOUNDING & MIXING TECHNIQUES**

[12L]



Rubber mixing mechanism, mixing machinery - Open mill mixing – Internal mixers – Continuous mixers – Factors affecting mixing – Flow behaviour of rubber compound, processibility test, Latex compounding and mixing. Troubleshooting.

**Unit III POSTCOMPOUNDING PROCESSING** [12L]

Calendaring: Sheetting – Skim coating – Fractioning – Topping – Doubling – Profiling – Spreading – Roll configurations – Control of thickness. Extrusion; Ram type – Screw type – L/D ratio and its influence – Hot & cold feed extruders – Pin barrel extruder – Twin screw extruder – Criteria for machine selection. Troubleshooting.

**Unit IV MOLDING & VULCANIZING TECHNIQUES** [12L]

**Molding:** Mold design, Compression, transfer and injection moulding – Blanks & pre-heating techniques, preparation of surfaces for bonding. Curing: Autoclaves, Hot air chambers, curing of built up articles, continuous vulcanization, L.C.M. (Liquid Curing Media), Fluidized Bed, microwave curing. Hand building and forming equipment for tank, pipe lining, roller covering. Troubleshooting.

**Unit V FINISHING OF RUBBER PRODUCTS** [12L]

Equipment's for flash and spew removal – Cryogenic techniques – Hand trimming – roller trim, buffing, tumbling, punching, grinding, shot blasting, painting, lacquering – Guards, Trip devices, Photoelectric and pressure sensitive devices – Maintenance of guards.

**References:**

1. Dr. B.R.Gupta, Rheology of Elastomers.
2. H.A.Barnes, J. F. Hutton and K. Walters, An Introduction to Rheology, Elsevier, 1989.
3. Rubber Processing, James L. White, Hanser Publishers, 1995.
4. C. M. Blow and C. Hepburn, Rubber Technology and manufacture, Butterworths, 1982.
5. C. W. Evans, Practical Rubber Compounding and processing, Applied Science, Publishers, London, 1981.
6. J. L. White, Rubber Processing Technology Materials, Principles, Hanser Publication, New York, 1995.
7. Kleemann, Weber, Elastomer Processing, Hansar, 2005.

**IPCHEM 353: TESTING OF RUBBER ALLIED MATERIALS & COMPOSITES**

**Unit I PRINCIPLES OF TESTING & RAW MATERIAL TESTING** [15L]

Principles of Testing, Standards and specification, Nomenclature- ISO and other standards, Laboratory Management System as per ISO/IEC 17025:2005 and Quality Management System as per ISO : 9001:2015.

Molecular weight distribution using GPC, Analysis of antioxidant, process oil and other additives by using GC GCMS, UV-Vis spectrophotometer, ICP-OES and DSC. Polymer identification by FTIR, Ash Content, Melting point, Moisture content and Specific gravity

### **Unit II TESTING OF RAW RUBBER & UN-VULCANIZED RUBBER COMPOUND**

[15L]

**Viscosity Characterization** – Brookfield Viscosity, Mooney viscosity,

Mass, Density, Dimensions Compression plastimeter, plasticity retention index, rotation plastimeters, extrusion rheometer, Scorch and cure rate: oscillating disk rheometer, moving die rheometer, rubber process analyzer etc.

### **Unit III TESTING OF VULCANIZATE**

[15L]

**Mechanical Properties** – Different types of Hardness, (Shore A, Shore D, IRHD and micro hardness) tear, tensile, compression, application of test data, abrasion resistance, Shear, Creep & Stress relaxation, Resilience, Aging and uniaxial, biaxial compression test.

**Thermal Analysis:** Instrumentation, Polymer Identification, Compositional analysis, volatile matter, Rubber, Polymer blends, C-black & ash estimation using Thermal Analysis (TGA). Glass transition, Heat capacity, Thermal history of polymers, State of cure studies by using DSC and Thermal Mechanical Analysis (TMA)

### **Unit IV PROCESS & QUALITY CONTROL**

[15L]

Effect of environment – Oxygen, heat, ozone and swelling media

Fatigue – Flex cracking and cut growth – Heat buildup **Dynamic mechanical testing of rubbers**—Storage modulus, loss modulus, Tan delta, Natural frequency, transmittance and damping factor.

Testing of rubber products like hoses, gaskets, automotive tubes, bearings, Testing of conveyor belts, V-belts and Mounts.

### **References:**

1. Standard - ISO / IEC 17025:2005
2. Standard – ISO 9001:2015
3. C. D. Craver and T. Provder, Polymer Characterization, ACS Advances in chemistry Series, Volume 227, 1990

4. J. S. Dick, Rubber Technology Compounding and testing for Performance, Hanser Publisher, 2001.

## ELECTIVE COURSES

### IPCHEM 354: EC-I: BIOPOLYMERS & BIO COMPOSITES

#### Unit I BIOPOLYMERS & BIODEGRADATION [15L]

**Biopolymers:** Classification, Biopolymers from natural origin and mineral origin, isolation, properties.

**Biodegradation:** Mechanism of biodegradation (polyesters, polycarbonates, polyvinyl alcohol, polyurethanes and polyether's) factors influencing biodegradation. Types of biodegradable polymers – properties and application.

#### Unit II CHARACTERIZATION & TESTING FOR BIODEGRADABILITY [15L]

Test methods and standards for bio-degradable plastics, Criteria used in evaluation of biodegradable plastics, Description of current test methods – Scanning test for ready biodegradability, Test for inherent biodegradability, Test for simulation studies, Other methods for assessing polymer biodegradability.

#### Unit III BIOCOMPOSITES [15L]

Definition- classification- natural bio, fibre and nano fillers as reinforcement, biodegradable/ bio-based resins as matrices. Properties of biocomposites. Applications in automobile & buildings.

#### Unit IV APPLICATIONS OF BIOPOLYMERS [15L]

Biopolymer Films, Biodegradable mulching, Advantages and Disadvantages, Chemical sensors – Biosensors, Functionalized Biopolymer Coatings and Films, Applications of biopolymers in horticulture Food Packaging, Functional Properties, safety and Environmental aspects, Shelf life, Films and coatings in Food Applications, Materials for edible films and coatings, Biopolymer coatings for paper and paperboard, Bio-nanocomposite films and coating **References:**

- 1) R. Smith, Biodegradable polymers for industrial applications, Woodhead Publishing Ltd, CRC Press, 2005.
- 2) A. J. Domb, J. Kost and D. M. Wiseman, Handbook of Biodegradable polymers, Harwood Academic Publishers, 1997.
- 3) R. P. Wool, X. S. Sun, Bio-Based Polymers and Composites, Elsevier, 2005.
- 4) A. S. Singha and V. K. Thakur, Green Polymer Materials, Studium Press, 2012.
- 5) A. K. Mohanty, M. Misra and L. T. Drzal, Natural Fibers, Bio Polymers and Bio Composites, CRC Press, 2005.

## **IPCHEM 355: EC-II: POLYMER NANO COMPOSITES**

### **Unit I COMPOSITES**

[15L]

Characteristics, advantages, and need of composites –Polymer composite materials, classification and theory of composite materials; Polymer matrices - thermoplastics and thermosetting plastics; Fiber reinforcement of elastomers - short and long fiber composites – Other additives

### **Unit II NANOMATERIALS USED IN POLYMERS**

[15L]

Nanofillers in bulk polymers - overview of potential nanostructured fillers - types - nanoparticles, nanofibers, nanotubes, nanosheets; surface features and layers and its modification. Techniques used to characterize nanostructured materials –XRD, AFM, etc.

### **Unit III CARBON NANOTUBES & THEIR APPLICATIONS**

[15L]

Structure of carbon nanotubes, processing methods for nanotube based polymer nanocomposites, nanotube alignment, characterization, properties and applications,

### **Unit IV PREPARATION & APPLICATION OF POLYMER NANO COMPOSITES**[15L]

Preparations of polymer nanocomposites - melt blending, solution blending, latex coagulation, in-situ polymerization, characterization, properties and application.

Polymers in nanoelectronics, Magnetic polymer nanocomposites, Wear resisting polymer nanocomposites, Packaging, Bio-medical, surface coatings, etc.

### **References:**

- 1) Yiu-Wing Mai and Zhong-Zhen Yu, Polymer Nanocomposites, Woodhead Publishing Limited, 2006.
- 2) K. Friedrich, S.Fakirov and Zhong Zhang, Polymer Composites from Nano to Macro, Springer 2005.
- 3) C.N.R.Rao, A.Muller, and A.K.Cheetham, The chemistry of Nanomaterials, Vol 1 & Vol.2, Wiley-VCH, 2005.
- 4) J. H. Kao, Polymer Nanocomposites, McGraw-Hill Publishers, 2006.

## **IPCHEM 356: INDUSTRIAL POLYMER CHEMISTRY PRACTICAL-I**

1. Preparation of Phenol formaldehyde resin – novolak and resol / polysulfide rubber
2. Determination of: acid value / hydroxyl value of given polymer sample
3. Determination of saponification value of given oil
4. Estimation of total alkalinity of the latex
5. Viscosity measurement by Brookfield viscometer

6. Molecular weight determination of polymer by GPC
7. Determination of volatile matter, dirt, ash content in Rubber from Natural sources
8. Estimation of Cu, Fe and Mn in rubber by ICP
9. Rubber identification pyrolysis and spot test by specific reagents (ASTM solution)
10. TGA of different rubber
11. DSC analysis of Rubber Compounds
12. Mixing behaviour of NR on two roll mill / carbon black filled NR / carbon black filled SBR / carbon black filled SBR & NR blend / carbon black filled EPDM / carbon black filled NBR
13. Extrusion characteristics of a filled rubber mix- NR Ex / SBR / NBR / EPDM
14. Calendaring of rubber mix

### **IPCHEM 357: INDUSTRIAL POLYMER CHEMISTRY PRACTICAL-II**

1. Identification and classification of natural rubber by using FTIR, Mooney, and other chemical methods.
2. Identification and classification of synthetic rubbers by using burning test, FTIR, Mooney, and other chemical methods.
3. Identification and classification of different type of carbon black
  - a. DBP absorption
  - b. IAN
  - c. Surface area Calculation
4. Identification and classification of rubber compounding materials, namely, **Zinc oxide / Stearic acid / Sulfur / Antioxidants / Accelerators / Processing oils**
5. Evaluation of tyre tread compound by using abrasion resistance index, heat build-up and DMA.
6. Evaluation of properties of seal & gasket rubber compound
7. Tyre testing by Endurance, rolling resistance, plunger energy, bead unseat etc.
8. Testing of: LPG Hose, Pressure cooker rubber gasket / Hose testing / Mount / Conveyor Belt / Condom / Tube
9. Design & development of : Tyre tread material / Hose cover / Conveyor belt cover / Gasket compound / footwear compound / latex dipped products / mounts / rubber mats / door profiles / tube compound
10. Curing Process of Rubber Compound- NR filled / SBR filled / NBR filled / EPDM filled / BR filled
11. Curing Process of Rubber Compound- by transfer molding technique

12. Curing Process of Rubber Compound- by injection molding technique of metal to rubber bonded products

13. Curing Process of Rubber mounts / Rubber Gaskets / Rubber Seals / Rubber Gauntlets

**SEMESTER-IV**

Course Code	Title of the Course	No. of Credits	No. of Hours	Examination		Total Marks
				Continuous Evaluation	End SEM	

IPCHEM 451	Design & Development of Rubber Products	04	60	40	60	100
IPCHEM 452	Latex Science & Adhesives	04	60	40	60	100
IPCHEM 453	Tyre Science and Technology	04	60	40	60	100
IPCHEM 454 OC- I	Intellectual Property Rights & Cheminformatics	04	60	40	60	100
IPCHEM 455 OC- II	Research Methodology	04	60	40	60	100
IPCHEM 456	Research Project	08	*	80	120	200

**No. of CREDITS: 24      TOTAL MARKS: 600**

**Students will have to select one of the optional courses i.e. IPCHEM 454 OC-I or  
IPCHEM 455 OC-II.**

**Practical component involves 16 hour per week of laboratory work for 15 weeks**

**SYLLABUS: SEMESTER-IV:**

**IPCHEM 451: DESIGN & DEVELOPMENT OF RUBBER PRODUCTS**

**Unit I FORMULATION DESIGN OF RUBBER COMPOUNDS**

**[15L]**

Basics of compounding, Approach for compounding, Selection of Rubbers, Fillers, Curing agents and Special additives in Rubber Compounding. Rubber compounds

feasibility for static and dynamic application, Rubber compounds for general purpose, oil resistant, heat resistant, fire resistant and weather resistance purposes.

**Unit IIDESIGN & DEVELOPMENT OF TYRES** [15L]

Different components of tyres and their compounding, Tyre materials & Tyre processing techniques.

**Unit III CONVEYOR BELT TECHNOLOGY** [15L]

Different types of conveyor belts, Mixing, Compounding and Calendaring, Building, Curing and Testing, Finishing and Packaging. **V-belt—Building**

**Unit IV PRODUCT DEVELOPMENT OF HOSES** [15L]

Different kind of hoses, Extrusion of cover, Reinforcement, curing by autoclave.

**References:**

1. Setright J.K., Automobile Tyres, Champan & Hall, 1972.
2. The Pneumatic Tire, (Ed) A N Gent & J D Walter, The University of Akron, August. 2005, published by NHTSA, DOT, USA
3. Elastomers: Criteria for Engineering Design, C Hepburn & R J W Reynolds, Applied Science Publishers, London, 1979.
4. Khairi Nagdi, Rubber as an Engineering Material: Guideline for Uses, Hanser Publishers, 1993.

**IPCHEM 452: LATEX SCIENCE AND ADHESIVES**

**Unit II LATEX SCIENCE** [15L]

Definition of Latex, classification, Latex particle size and distribution, stability and destabilization of latices, Comparison between latices and polymer solution. Characteristic and processing of natural rubber latex.

**Unit III LATEX APPLICATION** [15L]

Latex dipped products, latex foam rubber, latex thread, latex and textile based rubber products, latex based surface coating, latex and paper.

**Unit III RUBBER BASED ADHESIVES** [15L]

Natural rubber adhesive, butyl rubber and polyisobutylene, nitrile rubber adhesive, styrene butadiene rubber adhesive, thermoplastic rubber in adhesive, carboxylic polymers in adhesive, neoprene based solvent and latex adhesive, polysulfide sealant and adhesives

**Unit IV RESIN BASED REACTIVE ADHESIVES** [15L]

Phenolics, epoxies, acrylics, anaerobics, cyanoacrylates – Uses of adhesives in civil engineering, automobile, aerospace, electrical & electronic industries.

**References:**



1. D. C. Blackley, High Polymer Latices, Vol 1 and 2, Maclaren & Sons, 1966.
2. R. F. Mausser, The Vanderbilt Latex Hand book, 3rd Edn.
3. R. Waterman, R. F. Mausser & E. E. Miller, Vanderbilt Latex Book on Process and Compounding Ingredients, R T Vanderbilt Publishers.
4. K. O. Calvert, Polymer Latex and Applications, 1985.
5. I. Skiest (Ed), Hand book of Adhesives, Van Nostrand Reinhold, 1990.
6. Shields, Hand Book of Adhesives, Butterworths, 1984.

### **IPCHEM 453: TYRE SCIENCE AND TECHNOLOGY**

#### **Unit I TYRE STRUCTURE**

**[15L]**

A historical introduction on the design and development of tyres of various kinds and type the current status of tyre industry in India and its future prospects, tyre sizing and marking on the tyres, different types of tyres bias-belted tyre, tube and tubeless tyre, their basic functions and performance comparisons. Different components of a tyre, its geometry, basic functions. Functions of a pneumatic tyre-load carrying, vibration and noise reduction, tyre function as a spring, contribution to driving control and road adhesion, the tyre friction contribution to driving control, steering control and self aligning torque.

#### **Unit II TYRE CARCASS AND BUILDING**

**[15L]**

Manufacturing techniques of various tyres like two wheeler and car tyres, truck tyres, OTR, farm tyres, aircraft tyres. Principles of designing formulations for various rubber components. Tyre reinforcement materials (Textile, steel, glass etc.). Criteria of selection, different styles and construction, textile treatment. Tyremould design, green tyre design principles, methods of building green tyres for bias, bias belted, radial and tubeless tyres, green tyre treatments. Tyre curing methods, post cure inflation, quality control tests. Tyre related products, their design and manufacturing techniques, tubes, valvesflaps, bladders. Different types, their features and operation of tyre building machines, bead winding machine, wire/glass processing machines, bias cutters, curing presses.

#### **Unit III[15L]**

Tyre wear, rubber friction and sliding mechanism, various factors affect- ing friction and sliding. Tyre stresses and deformation, tyre noise, mechanism of noise generation, effect of tread pattern, vehicle speed etc. onTyre wear, rubber friction and sliding mechanism, various factors affect- ing friction and sliding. Tyre stresses and deformation, tyre noise, mechanism of noise generation, effect of tread pattern, vehicle speed etc. on

#### **Unit IV TESTING OF TYRE**

**[15L]**

Measurement of tyre properties, dimension and size-static and loaded. Tyre construction analysis, endurance test, wheel and plunger tests, traction, noise measurements. Force and moment characteristics, cornering coefficient, aligning torque coefficient, load sensitivity and load transfer sensitivity. Rolling resistance, non uniformity, dimensional variations, force variations, radial force variation, lateral force variation, conicity and plysteer. Tyre, balance, mileage, evaluations. Tyre flaws and separations. X-ray holography etc. Foot print pressure distribution. BIS standards for tyres, tubes and flaps.

### **References:**

1. TyreScience&Technology (Journal oftheTyreSociety) Akron,Ohio.
2. Tyre Technology 'Tom French', Adam Higher, New York.
3. Tyre Mechanics & Testing (Sponsored Course, Feb. '83) Roorke....
4. Mechanics of Pneumatic Tyres, Samuel C Lark, US Department of Transportation Washington. .
5. (a) Year Book, (b) Engineering Design Informations, The Tyre& Rim Association.
6. Tyre, Valve & Rim data, ITTAC, New York.
7. LJK Setright. "Automobile Tyres". Chapman & Hall, London.
8. Tyre Technology, F.J.Kovac, GOODYEAR Tyre and Rubber Com- pany, USA.

## **OPTIONAL COURSES**

### **IPCHEM 454 OC-I: INTELLECTUAL PROPERTY RIGHTS & CHEMOINFORMATICS**

#### **Unit-I [15L]**

##### **Introduction to Intellectual Property: [2L]**

Historical Perspective, Different types of IP, Importance of protecting IP.

##### **Patents: [5L]**

Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.

##### **Industrial Designs: [2L]**

Definition, How to obtain, features, International design registration.

##### **Layout design of integrated circuits: [2L]**

Circuit boards, Integrated Chips Importance for electronic industry.

##### **Copyrights: [2L]**

Introduction, How to obtain, Differences from Patents.

##### **Trade Marks: [2L]**

Introduction, How to obtain, Different types of marks-Collective marks, certification marks, service marks, Trade names, etc.

#### **Unit-II[15L]**

##### **Geographical Indications: [2L]**

Definition, rules for registration, prevention of illegal exploitation, importance to India.

**Trade Secrets:** [2L]

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

**IP Infringement issue and enforcement:** [5L]

Role of Judiciary, Role of law enforcement agencies-Police, Customs, etc.

**Economic Value of Intellectual Property:**

Intangible assests and their valuation, Intellectual Property in the Indian Context- Various Laws in India Licensing a technology transfer.

**Different International agreements:** [6L]

**(a) World Trade Organization (WTO):**

- (i) General Agreement on Tariffs & Trade (GATT) , Trade Related Intellectual Property Rights (TRIPS) agreement
- (ii) General Agreement on Trade related Services (GATS)  
Madrid Protocol
- (iii) Berne Convention
- (iv) Budapest Treaty

**(b) Paris Convention**

**WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity**

**Unit-III**[15L]

**Introduction to Cheminformatics:** [5L]

History and evolution of cheminformatics, Use of cheminformatics, Prospects of cheminformatics, Molecular Modeling and Structure elucidation.

**Representation of molecules and chemical reactions:** [5L]

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

**Searching chemical structures:** [5L]

Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

**Unit-IV** [15L]

**Applications:**

Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure-Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure-Spectra correlations, Prediction of NMR, IR and Mass spectra, Computer Assisted Structure

elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, Analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-Based and Structure Based Drug Design, Application of Cheminformatics in Drug Design.

**Reference books:**

1. Andrew R. Leach & Valerie, J. Gillet, (2007), *An introduction to Cheminformatics*. Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: a text-book*. Wiley-VCH.
3. Gupta, S.P. *QSAR and Molecular Modeling*, Springer-Anamaya Pub.: New Delhi.

**IPCHEM 455 OC-II: RESEARCH METHODOLOGY**

**Unit-I-LITERATURE SURVEY [15L]**

**Print:**

[5L]

Primary, Secondary, Tertiary sources,

**Journals:**

Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, SubjectIndex, Substance Index, Author Index, Formula Index, and other Indices with examples.

**Digital:**

[5L]

Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-Databases, ChemSpider, Science Direct, SciFinder, Scopus.

**Information Technology and Library Resources:**

[5L]

The Internet and World Wide Web, Internet resources for chemistry, Finding and citing published information.

**Unit-II-DATA ANALYSIS [15L]**

**The Investigative Approach:**

Making and recording Measurements, SI Unit-s and their use, Scientific methods and design of experiments.

**Analysis and Presentation of data:**

Descriptive statistics, Choosing and using statistical tests, Chemometrics, Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit,  $r$  and its abuse, Basic aspects of multiple linear regression analysis.

### **Unit-III METHODS OF SCIENTIFIC RESEARCH & WRITING SCIENTIFIC PAPERS [15L]**

Reporting practical and project work, Writing literature surveys and reviews, Organizing a poster display, Giving an oral presentation.

#### **Writing scientific papers:**

Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, Writing ethics, Avoiding plagiarism.

### **Unit IV: CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS [15L]**

Safe working procedure and protective environment, protective apparel, emergency procedure, and first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric- safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

#### **Reference books:**

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), *Practical skills in chemistry*, 2<sup>nd</sup> Ed., Prentice Hall, Harlow.
2. Hibbert, D. B., & Gooding, J. J., (2006), *Data analysis for chemistry*, Oxford University Press.
3. Topping, J., (1984), *Errors of observation and their treatment*, 4<sup>th</sup> Ed. Chapman Hill, London.
4. Harris, D. C., (2007), *Quantitative chemical analysis*, 6<sup>th</sup> Ed., Freeman Chapters 3-5
5. Levie, R. de., (2001), *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ Press 487 pages.
6. Chemical safety matters-IUPAC-IPCS, Cambridge University Press, 1992.
7. OSU safety manual 1.01

### **IPCHEM 456: RESEARCH PROJECT**

Each student will be assigned a project involving some design and fabrication work, as well as

Theoretical and Experimental studies on some problem related to Rubber and Plastics

Technology. Continuous internal assessment marks for the project will be given during Project

Review meeting. The student has to prepare and present a detailed project report at the end of the semester and give a presentation about the work done. End semester examination mark will include viva voce examination.