University of Mumbai

DEPARTMENT OF CHEMISTRY

(AUTONOMOUS)

FOR M. Sc. AND Ph. D. DEGREE PROGRAMMES IN CHEMISTRY

DEPARTMENT OF CHEMISTRY
UNIVERSITY OF MUMBAI
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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 SEMESTE-R	Examination		Total Marks
				Mid Sem Marks	End-Sem Marks	
CHEM 101	Physical Chemistry I	4	60	40	60	100
CHEM 102	Inorganic Chemistry I	4	60	40	60	100
CHEM 103	Organic Chemistry I	4	60	40	60	100
CHEM 104	Analytical Chemistry I	4	60	40	60	100
CHEM 105	Physical Chemistry Practical I	2	-	-	50	50
CHEM 106	Inorganic Chemistry Practical I	2	-	-	50	50
CHEM 107	Organic Chemistry Practical I	2	-	-	50	50
CHEM 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

CHEM 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-IV CHEMICAL 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*, 7th ed., Oxford University Press, 2002.
2. K. J. Laidler and J. H. Meiser, *Physical Chemistry*, 2nd ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rd ed., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5th ed., Tata McGraw-Hill, New Delhi, 2002.
5. G. W. Castellan, *Physical Chemistry*, 3rd 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, 2nd 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*, 2nd 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*, 3rd 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*, 5th 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*, 5th ed., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
6. J. P. Lowe, *Quantum Chemistry*, 2nd 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.

CHEM-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 (BeH_2); sp^2 (BF_3); sp^3 (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 pKa 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. Banerjea, Coordination Chemistry, Tata McGraw Hill, 1993.
2. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd 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, 5th 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, 5th Ed., Wiley Interscience, 2009.
2. R. C. Mehrotra and A. Singh, Organometallic Chemistry-A Unified Approach, 2nd 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, 2nd Ed., John Wiley & Sons, 1983.
6. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4th Ed., Harper Collins, 1993.

Unit-III

1. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4th 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 BenjaminCummings Publishing Company, 1989.
4. K. L. Kapoor, A textbook of Physical Chemistry, Volume 4, McMillan, 2001.
5. G. Miessler and D. Tarr, Inorganic Chemistry, 3rd 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, 2nd 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, 3rdEd., John Wiley & Sons, Inc., 2001.
3. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5thEd., Oxford University Press, 2010.
4. G. Miessler and D. Tarr, Inorganic Chemistry, 3rd 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, 4th Ed., Harper Collins, 1993.
7. R. L. Madan and G. D. Tuli, Inorganic Chemistry,5th Ed., S. Chand, 2012.
8.. J. D. Lee, Concise Inorganic Chemistry, 5th 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

CHEM 103: ORGANIC CHEMISTRY-I

Unit-IPHYSICAL ORGANIC CHEMISTRY [15L]

1.1Acidity-Basicity:

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

1.2Non-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.

1.3Linear 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: Symmertry operations and symmetry elements:

Symmetry Operations, identification of principal axis, symmetry elements, definition and examples of molecules with different elements of symmetry including σ_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 enatiotopic, 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 FUNCTON [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- IVSPECTROSCOPY [15L]

4.1 UV-Visible Spectroscopy:

Recapitulation of basic concepts and sample handling. Woodward-Fieser rules for calculation of λ_{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 mechamism, 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, 6th edition onwards.
20. Physical Organic Chemistry, Neil Isaacs
21. Modern Physical Organic Chemistry, Eric V. Anslyn and Dennis A. Dougherty

CHEM 104: ANALYTICAL CHEMISTRY I

Unit I: Concepts of Analytical Chemistry **[15L]**

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]

Unit II: Atomic and molecular spectroscopy **[15L]**

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]

UNIT III: Separation methods **[15L]**

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]

UNIT IV: Column chromatography techniques **[15L]**

4.1 Gas Chromatography: Principle of GLC and GSC; Instrumentation: carrier gas supply, sample introduction systems, packed & capillary columns; choice of detectors and comparative account of TCD, FID, ECD & thermionic detector. [4L]

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*, 5th ed., Philadelphia: Saunders College Publishing, 1998.
2. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 8th ed., Philadelphia: Saunders College Publishing, 2004.
3. G. D. Christian, *Analytical Chemistry*, 6th 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*, 6th 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*, 6th 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*, 3rd 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*, 9th 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, 2th ed. ELBS.
17. R. A. Day, Jr. and A. L. Underwood, *Quantitative Analysis*, 6th 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,* 3rd 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 2nd edition.* WILEY-VCH 2004.
21. Solid phase Extraction- Principles, Techniques and Applications, N. J. K. Simpson, Marcel Dekker, New York, (2000).

CHEM 105: PHYSICAL CHEMISTRY PRACTICAL-I

Instrumental Experiments:

Conductometryand 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 iso-electric point of the acid.

CHEM-106: INORGANIC CHEMISTRY PRACTICAL-I

Synthesis, Purification and Analysis of the following Inorganic Preparations:

1. Potassium trioxalatochromate (III)
2. Bis(enthylenediammine) copper (II) sulphate
3. Hexammine nickel (II) chloride/sulphate
4. Potassium dioxalato cuprate(II) dihydrate
5. Potassium trioxalatoaluminate(III) hydrate

Reference books:

1. A. I. Vogel, Vogel's Text Book of Quantitative Inorganic Analysis, 6th 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 Nostrnad Reinhond, 1972.
7. G. Pass and H. Sutcliffe, Practical Inorganic Chemistry, 2nd Ed., Chapman and Hall, 1985.

CHEM 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 preaparations 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.)

CHEM 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 SEMESTE-R	Examination		Total Marks
				Mid Sem Marks	End-Sem Marks	
CHEM 201	Physical Chemistry II	4	60	40	60	100
CHEM 202	Inorganic Chemistry II	4	60	40	60	100
CHEM 203	Organic Chemistry II	4	60	40	60	100
CHEM 204	Analytical Chemistry II	4	60	40	60	100
CHEM 205	Physical Chemistry Practical II	2	-	-	50	50
CHEM 206	Inorganic Chemistry Practical II	2	-	-	50	50
CHEM 207	Organic Chemistry Practical II	2	-	-	50	50
CHEM 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

CHEM 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 (ψ) 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*, 7th ed., Oxford University Press, 2002.
2. K. J. Laidler and J. H. Meiser, *Physical Chemistry*, 2nd ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rd ed., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5th ed., Tata McGraw-Hill, New Delhi, 2002.
5. G. W. Castellan, *Physical Chemistry*, 3rd 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, 2nd 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*, 5th ed., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
11. J. P. Lowe, *Quantum Chemistry*, 2nd 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*, 2nd 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*, 4th 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*, 2nd 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*, 3rd 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*, 5th ed., John Wiley and Sons, Inc., 1994.
3. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.

CHEM-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_2 [fluorite (CaF_2), antifluorite (Na_2O), rutile (TiO_2) and layer structures viz., cadmium chloride ($CdCl_2$) and cadmium iodide, (CdI_2)].

(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, 2nd Ed., Cambridge University Press, 1997.
5. Lesley E. Smart and Elaine A. Moore, Solid State Chemistry – An introduction, 3rd 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, 2nd Ed., New Age International Publishers2009.
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, 2nd Ed., Wiley Eastern Ltd., 1989.
5. G. Raj, A. Bhagi and V. Jain, Group Theory and Symmetry in Chemistry, 3rd Ed., Krishna Prakashan, 2010.
6. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5th 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, 7th Ed., New Age International Publishers, 2007.
2. G. S. Sodhi, Fundamental Concepts of Environmental Chemistry, 3rd Ed., Narosa Publishing House, 2013.
3. S. S. Dara and D. D. Mishra, A Textbook of Enviromental 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, 2nd 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, 2nd Ed., Academic Press, 2005.
7. J. E. Girard, Principles of Environmental Chemistry, 2nd Ed., Jones and Bartlett publishers, 2011.

8. H. Kaur, Environmental Chemistry, Pragati Prakashan, 8th Ed., 2014.

Unit-IV

1. I. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, Bioinorganic Chemistry, 1st 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, Caligronic, 1994.
6. G. N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, Dhuri & Sons, 1988.

CHEM 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\s 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-Muslin diagrams, Huckel's (4n+2) π electron rule, Exceptions to (4n+2) π 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-IIELIMINATION AND NUCLEOPHILIC SUBSTITUTION REACTIONS

[15 L]

2.1 Types of elimination reactions, $E_1$and E_2mechanisms.

2.2 Orientation of elimination reactions: Saytzeff and Hoffmann rules. E_2reactions of vinyl halide, E_1cB mechanism.

2.3 Pyrrolytic elimination: Chugaev reaction, Cope reaction, Hoffmann's and Pyrrolysis of acetates.

2.4 Aliphatic nucleophilic substitution at sp^3 carbon: S_N1, S_N2, S_Ni, S_NcA reactions. Ion pair in S_N1, 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^2 (vinylic) carbon.

2.6 Aromatic nucleophilic substitution reaction: S_NAr, S_N1,Benzynemechanism, ipso, cine and tele substitutions, vicarious substitution.

Unit-III OXIDATION-REDUCTION [15 L]

3.1Preparation 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

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

Wolf-Kishner reduction, Clemmensen reduction, Meerwein-Pondorff-Verley reduction, Birch reduction, Reductions with $NaBH_4$, $LiAlH_4$and DIBAL.

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

Unit-IVREACTIONS 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 mechamism, 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, 6th 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.

CHEM 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*, 5th ed., Philadelphia: Saunders College Publishing, 1998.
2. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 8th ed., Philadelphia: Saunders College Publishing, 2004.
3. G. D. Christian, *Analytical Chemistry*, 6th 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*, 6th 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*, 6th 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,* 3rd 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*, 9th 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, 2th ed. ELBS.

17.R. A. Day, Jr. and A. L. Underwood, *Quantitative Analysis,* 6th 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,* 3rd 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 2nd edition.* WILEY-VCH 2004.

CHEM 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 $KI + I_2 \quad KI_3$ by distribution method.
7. Investigation of the reaction between acetone and iodine.

CHEM-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, 6th 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 Nostrnad Reinhond, 1972.
7. G. Pass and H. Sutcliffe, Practical Inorganic Chemistry, 2nd Ed., Chapman and Hall, 1985.

CHEM 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)

CHEM 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: PHYSICAL CHEMISTRY

Course Code	Title of the Course	No. of Credits	No. of hours per SEMESTER	Examination		Total Marks
				Continuous Evaluation Marks	End-Sem Marks	
CHEM 311	Solid State Chemistry	4	60	40	60	100
CHEM 312	Spectroscopy	4	60	40	60	100
CHEM 313	Statistical thermodynamics, thermodynamics of biological systems & electrochemistry-I	4	60	40	60	100
CHEM 314 EC-I	Interfacial Science	4	60	40	60	100
CHEM 315 EC-II	Some Selected Topics in Physical Chemistry	4	60	40	60	100
CHEM 316	Physical Chemistry Practical III	4	-	-	100	100
CHEM 317	Physical Chemistry Practical IV	4	-	-	100	100

No. of CREDITS: 24 TOTAL MARKS: 600

Students will have to select one of the electives i.e. CHEM 314 or CHEM 315

Practical component involves 16 hr per week of laboratory work for 15 weeks.

SEMESTER-III: PHYSICAL CHEMISTRY

CHEM 311: SOLID STATE CHEMISTRY

Unit-I: BONDING, STRUCTURE AND PREPARATIVE METHODS [15L]

Bonding and Structure: Classification of solids based on nature of forces (Ionic, Covalent, Metallic, van der Waals, Hydrogen-bonded), Crystal Structures: Symmetry and Choice of Unit- cell, Bravais lattice, Miller indices, Point groups and space groups, Close packing, Lattices and Unit- cells, Crystalline solids, ionic radii, radius ratio rule, lattice energy, crystal structure determination by powder diffraction and single crystal X-ray diffraction.

Preparative Methods: Solid state reactions (General Principles, precursor methods), Crystallization of solutions, melts, glasses and gels, vapour phase transport methods, Preparation of thin films, growth of single crystals, high pressure and hydrothermal methods.

Some important solid-state materials: Magnetoresisters, Zeolites, Intercalation compounds, fullerides.

Unit-II: DEFECTS AND DIFFUSION IN SOLIDS [15L]

Defects and non-stoichiometry: Types of Defects: Point defects, plane defects, line defects. Thermodynamics of defects, Solid solutions.

Diffusion in solids: Mechanisms, Steady state and non-steady state diffusion, factors affecting diffusion, Kirkendall effect.

Unit-III: ELECTRICAL AND MAGNETICPROPERTIES [15L]

Electrical Properties:

Electrical conductivity of metals, Free electron theory, semiconductors, Intrinsic and extrinsic semiconductivity, Band theory, Superconductivity: Conventional Superconductors, Bardeen-Cooper-Schrieffer (BCS) theory, High temperature Superconductors, Ferromagnetic Superconductors, Uses of High temperature Superconductors.

Magnetic Properties:

Diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism, ferrimagnetism. Calculation of magnetic moments, influence of temperature on magnetic behaviour, domains and hysteresis, Soft and hard magnetic materials.

Unit-IV: OPTICAL PROPERTIES, DIELECTRIC PROPERTIES AND PHASE TRANSFORMATIONS IN SOLIDS [15L]

Optical Properties:

Electron emission in Metals, Photovoltaic effect, Luminescence, Laser and Maser actions, The Ruby laser, Light emitting diodes, Optical fibers.

Dielectric Properties:

Dielectric constant, Clausius-Mosotti equation, Piezoelectricity, Ferroelectricity, Antiferroelectricity, Ferrielectricity.

Phase transformations in solids:

Buerger's classification, Thermodynamic classification, Kinetics of phase transitions, temperature and pressure induced transformations, Martensitic transformations, Order-disorder transitions.

*** Numericals/Problems are expected from each Unit-**

Reference books:

1. H. V. Keer, *Principles of the Solid State*, New Age International Publishers,
2. A. R. West, *Solid State Chemistry and its Applications*, John Wiley and Sons (Asia) Pte. Ltd.,
3. L. E. Smart and E. A. Moore, *Solid State Chemistry – An Introduction*, 3rd Ed., Taylor and Francis, 2005.
4. V. Raghavan, *Materials Science and Engineering*, Fifth Ed., Prentice-Hall of India Pvt. Ltd., New Delhi, 2004.
5. William D. Callister, Jr., *Materials Science and Engineering, An Introduction*, Fifth Ed., John Wiley and Sons (Asia) Pte. Ltd., 2001.
6. S. O. Pillai, *Solid State Physics*, Fifth Ed., New Age International Publishers, 2002.
7. Leonid V. Azaroff, *Introduction to Solids*, Tata-McGraw-Hill Publishing Co. Ltd., New Delhi, 1977.
8. Sandra E. Dann, *Reactions and Characterization of Solids*, Royal Society of Chemistry, 2000.

CHEM 312: SPECTROSCOPY

Unit-I **BASIC PRINCIPLES OF SPECTROSCOPY** **[15L]**

Absorption and Emission of Radiation, Width and intensity of spectral lines, transition probability and selection rules, Fourier transform spectroscopy, computer averaging of signals (CAT), lasers.

Microwave spectroscopy: Rotational spectra of diatomic (non-rigid) molecules, Population of rotational levels and intensity of rotational lines, effect of isotopic substitution, rotational spectra of polyatomic molecules (linear and symmetric top), Stark effect.

Unit-II **INFRARED SPECTROSCOPY** **[15L]**

Anharmonic oscillator, Rotational-vibrational spectrum, Breakdown of Born-Oppenheimer approximation, combinational differences, vibrations of polyatomic molecules, rotational fine structure of vibrational spectrum of polyatomic molecules.

Raman spectroscopy:

Classical and quantum theory of Raman scattering, Experimental

Methods, Pure rotational, vibrational and rotational-vibrational Raman spectrum of diatomic and polyatomic molecules, polarization and depolarization of Raman lines, correlation of infrared and Raman spectra, normal modes and symmetry, Resonance Raman Scattering, Surface Enhanced Raman Scattering

Unit-III **ELECTRONIC SPECTROSCOPY:** **[15L]**

Vibrational course structure, Progressions and sequences, The Franck-Condon principle, Deslandres tables, Dissociation energies, Birge-Sponer extrapolation, Rotational fine structure, Fortrat diagram, Predissociation, Electronic spectra of polyatomic molecules.

Nuclear magnetic resonance spectroscopy: Chemical shift, spin-spin coupling, Chemical and magnetic equivalence, first and second order spectra, pulsed NMR, relaxation times, multipulse techniques, spin echoes, two- and three- dimensional NMR, NMR of nuclei other than proton, nuclear overhauser effect.

Unit- IV **NUCLEAR QUADRUPLE RESONANCE:** **[15L]**

Principle, Transitions for axially and non-axially symmetric systems, applications.

Electron spin resonance spectroscopy:

Basic theory, Instrumental Aspects, The *g* – factor, hyperfine structure, applications to free radicals, inorganic radicals, transition metal complexes.

Mössbauer Spectroscopy:

Principles, Recoilless emission and absorption of γ-rays, experimental methods, isomer shift, hyperfine structure (quadrupole interaction), magnetic hyperfine interaction, applications.

Reference books:

1. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata-McGraw-Hill, 1994.
2. M. L. Gupta, *Atomic and Molecular Spectroscopy*, New Age International Publishers, 2001.
3. H. S. Randhawa, *Modern Molecular Spectroscopy*, McMillan India Ltd., 2003
4. G. Aruldas, *Molecular Structure and Spectroscopy*, Prentice-Hall of India, 2001.
5. J. Michael Hollas, *Modern Spectroscopy*, 4th Ed., John Wiley and Sons, 2004.

List of Books for further reading:

1. R. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.
2. B. P. Straughan and S. Walker (Eds.), Spectroscopy – Vol 1-3, Chapman and Hall, New York, 1976.
3. R. K. Harris, *Nuclear Magnetic Resonance Spectroscopy*, Pitman, London, 1983.
4. Donald L. Pavia, Gary M. Lampman and George S. Kriz, *Introduction to Spectroscopy*, 3rd ed., Thomson, Brooks/Cole, 2001.

CHEM 313: STATISTICAL THERMODYNAMICS, THERMODYNAMICS OF BIOLOGICAL SYSTEMS & ELECTROCHEMISTRY-I

Unit-I **FUNDAMENTALS OF STATISTICAL THERMODYNAMICS** **[15L]**

Permutations, probability, microstates and configurations, the most probable distribution, ensembles, distribution laws: Boltzmann distribution, Bose-Einstein statistics, Fermi-Dirac statistics. Partition function, evaluation of translational, rotational, vibrational and electronic partition functions for ideal gases

Unit- II **APPLICATIONS OF STATISTICAL THERMODYNAMICS IN CHEMICAL SYSTEMS** **[15L]**

Calculation of thermodynamic properties (Energy, Heat capacity, Enthalpy, Entropy, Helmholtz energy, Gibbs energy) in terms of partition functions for mono, di and polyatomic gases, equilibrium constants, residual entropies, heat capacities of ideal gases, heat capacities of solids.

Unit-III **THERMODYNAMICS OF BIOLOGICAL SYSTEMS** **[15L]**

Thermodynamics of biopolymer solutions, thermodynamics of biochemical reactions involving adenosine triphosphate (ATP), osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechano-chemical systems.

Structures and functions of cell membrane, ion transport through cell membrane and irreversible thermodynamic treatment of membrane transport.

Biological Buffers.

Unit-IV **ELECTROCHEMISTRY-I** **[15L]**

Batteries: Working principle, cell reactions and cell performances of Lithium Batteries (Primary and secondary), Lithium and Lithium ion batteries.

Fuel cells: Classification, H_2–O_2 fuel cell, choice of electrolyte, advantages, disadvantages.

Electroplating: Electroplating of metals, factors affecting throwing power of an electroplating bath, mechanism of electro-deposition, typical electroplating processes and applications of electroplating metal.

Electrochemical corrosion of metals: Classification of corrosion processes, conditions for the occurrence of corrosion process, kinetic theory of corrosion and its application to pure metals, methods of corrosion protection, corrosion of technical metals.

Reference books:

1. D. A. McQuarrie and J. D. Simon, *Molecular Thermodynamics*, Viva Books Private Limited, First Indian Ed., 2004.

2. D. A. McQuarrie and J. D. Simon, *Physical Chemistry, a Molecular Approach*, Viva Books Private Limited, First South Asian Ed., 1998. Chap.
3. E. D. Kaufmann, *Advanced Concepts in Physical Chemistry*, McGraw-Hill, 1966.
4. Robert P. H. Gasser and W. Graham Richards, *An Introduction to Statistical Thermodynamics*, World Scientific Publishing Co. Pte. Ltd., 1995.
5. William Blum and George B. Hogaboom, *Principles of Electroplating and Electroforming*, 3rd ed., McGraw-Hill Book Co., 1949.
6. Frederick A. Lowenheim, *Modern Electroplating*, 3rd ed. John Wiley Sons, Inc., 1974.
7. L. I. Antropov, *Theoretical Electrochemistry*, Mir Publishers, Moscow, 1972.
8. H. H. Uhlig and R. W. Rewic, *Corrosion and Corrosion Control*, John Wiley and Sons, New York, 1985.
9. Mars G. Fortana, *Corrosion Engineering*, 3rd ed., McGraw-Hill Book Co., 1987.
10. Nester Perez, *Electrochemistry and Corrosion Science*, Kluwer Academic Publisher, 2004.
11. R. Narayan and B. Vishwanathan, *Chemical and Electrochemical Energy Systems*, Universities Press (India) Ltd., 1998.
12. C. R. Cantor and P. R. Schimmel, *Biophysical Chemistry*: Part I, II and III, W. H. Freeman and Co., 1980.
13. R. B. Martin, *Introduction to Biophysical Chemistry*, McGraw-Hill New York, 1964.
14. S. Ramakrishnan, *Biophysical Student Mannual*, T. R. Publications (Madras), 1994.
15. J. H. Weil, *General Biochemistry*, New Age International Publishers, New Delhi.

CHEM 316: PHYSICAL CHEMISTRY PRACTICAL-III

Major Experiments

Distribution Methods:

1.To determine the formula of copper ammonia complex.

2.To determine the formula of silver ammonia complex.

Phase Equilibrium:

1.To determine the freezing point curve of two component simple eutectic system.

2.To determine the freezing point curve of two component compound forming system.

Reaction Kinetics:

1. To study the kinetics of hydrolysis of methyl acetate catalyzed by hydrochloric acid at different temperatures and to determine the thermodynamic parameters.
2. To study the influence of ionic strength on the rate of reaction between potassium persulphate and potassium iodide in solution.
3. To study the kinetics of reaction between potassium persulphate and potassium iodide in solution at different temperatures and determine the thermodynamic parameters.

CHEM 317: PHYSICAL CHEMISTRY PRACTICAL-IV

Minor Experiments

Solubility:

Study the variation of solubility of calcium hydroxide in the presence of sodium hydroxide and hence determine the solubility product at room temperature.

Viscosity Measurements:

1. To determine limiting viscosity number of polystyrene.
2. To determine chain linkage in polyvinyl alcohol from viscosity measurements.
3. To determine relative molecular mass of polystyrene from viscosity measurements.

Surface Chemistry:

1. To determine the critical micelle concentration (CMC) of sodium lauryl sulphate/N-cetyl-N,N,N-trimethyl ammonium bromide (CTAB) from measurements of conductivities at different concentrations.
2. To determine the critical micelle concentration (CMC) of sodium lauryl sulphate/N-cetyl-N,N,N-trimethyl ammonium bromide (CTAB) from measurements of surface tensions at different concentrations.

Potentiometry / pH metry:

1. To determine the stability constant of the silver-ammonia complex.
2. To determine the transport number of silver and nitrate ions in aqueous solution from the cell potential of the concentration cell with liquid junction potential.
3. To determine the substitution constants in Hammett equation for 3-aminobenzoic acid/4-aminobenzoic acid and 3-nitrobenzoic acid/4-nitrobenzoic acid.

Spectrophotometry:

1. To determine the ionization constant of methyl red/ bromophenol blue.

Interpretation of spectra/data-I:

1. Interpretation of vibrational-rotational spectra of rigid and non-rigid diatomic molecules
2. Interpretation of electronic spectra of diatomic molecules.
3. Interpretation of electronic spectra of simple polyatomic molecules.
4. Interpretation of ESR spectra.
5. Interpretation of Mössbauer spectra.
6. Analysis of XRD pattern of cubic system
7. Interpretation of DTA, TG, DTG curves.

Interpretation of spectra/data-II:

Spectral analysis: Structure elucidation with a given set of spectra, Determination of the degree of un-saturation from molecular formula. Systematic interpretation of set of spectra including some or all of the following: UV-Vis, IR, PMR, CMR, DEPT, Mass. Identification of the compound based on systematic interpretation of spectral data would be preferred.

List of reference Books for Practicals and Spectral Interpretaion:

1. B. Vishwanathan and P. S. Raghavan, Practical Physical Chemistry, Viva Books Private Limited, 2005.
2. A. M. James and F. E. Prichard, *Practical Physical Chemistry*, 3rd ed., Longman, 1974.
3. B. P. Lewitt (ed.), *Findlay's Practical Physical Chemistry*, 9th ed., 1973.
4. C. D. Brennan and C. F. H. Tipper, *A Laboratory Manual of Experiments in Physical Chemistry*, McGraw-Hill, 1967.
5. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata-McGraw-Hill, 1994.
6. *Introduction to Spectroscopy*, Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks.
7. *Spectrometric Identification of Organic Compounds*, R. Silverstein, G.C Bassler and T.C. Morrill, John Wiley and Sons.
8. *Organic Spectroscopy*, William Kemp, W.H. Freeman & Company.
9. *Organic Spectroscopy-Principles and Applications*-Jagmohan, Narosa Publication.
10. *Organic Spectroscopy*, V.R. Dani, Tata McGraw Hill Publishing Co.
11. *Spectroscopy of Organic Compounds*, P.S. Kalsi, New Age International Ltd.
12. *Organic Structures from Spectra*, 4th ed., L. D. Field, S. Sternhell and J. R. Kalman, Wiley.

ELECTIVE COURSES

CHEM 314: EC-I: INTERFACIAL SCIENCE

Unit-I **HETEROGENEOUS CATALYSIS** **[15L]**

Adsorption on solid surfaces, Chemisorption at metal surfaces and oxides, Kinetics of catalyst reactions, structure, preparation and uses of heterogeneous catalysts, Application of catalysis in energy conversion, petroleum industry and atmospheric pollution control.

Unit-II **CATALYSIS AND GREEN CHEMISTRY** **[15L]**

Comparison of catalyst types, heterogeneous catalysts, zeolites-composition and structures, synthesis of zeolites, structure determination, uses of zeolites, zeolites as catalyst, zeolites and the bulk chemical industry, catalysts in fine chemicals and pharmaceutical industries, catalytic converters, homogeneous catalysts -transition metal catalysts with phosphine ligands-Wilkinson's Catalyst, greener Lewis acids, asymmetric catalysis, phase transfer catalysis, bio catalysis, photo catalysis.

Unit-III **NANOCHEMISTRY** **[15L]**

Introduction, Properties of materials & nanomaterials, role of dimensions in nanomaterials, advantages of nanosize over micron size, need of surface/encapsulation of nanomaterials, some important properties of nanomaterials, Techniques for synthesis of nanomaterials- Physical method and chemical method.

Nanocomposites:

Comparison with conventional composites. Manufacture and Characteristics of thermoplastic and thermoset nanocomposites products: Fibre reinforced nanocomposites, copolymer / clay nanocomposites, latex / ZnO nanocomposites, hybrid nanocomposites, PVC / CaCO3 nanocomposites, etc. Effect of modifier concentration on structure, mechanical and viscoelastic properties of nanocomposites, Development and Optimization of Polymer melt process, Nanocomposites preparation by injection moulding

Unit-IV **SURFACE CHARACTERIZATION TECHNIQUES** **[15 L]**

Principles, instrumentation and applications of:

Electron spectroscopy: ESCA, AUGER and UPS.

Electron microscopy: Scanning electron microscopy, Scanning probe microscopes: The Scanning Tunneling Microscope, Atomic force Microscope.

Reference Books:

1. R.P.W.Scott, *Tandem Techniques*, Wiley India Pvt.Ltd. Reprint 2009.
2. J. Barker, *Analytical chemistry for open learning, Mass spectrometry*, Wiiley IndiaED.
3. H. J. Arnikar, *Essential of Nuclear Chemistry*, New Age International, 1995.
4. G. C. Bond, *Heterogeneous Catalysis*, 2nd ed., Clarendon Press, Oxford, 1987.
5. Mike Lancaster, Green Chemistry: An Introductory Text, Royal Society of Chemistry, 2002.
6. Paul T. Anastas and John C. Warner, Green Chemistry – Theory and Practice, Oxoford University Press, 1998.
7. Albert S. Matlack, Introduction to Green Chemistry, Marcel Dekker, Inc., 2001.
8. Text/Reference books
9. Novel Nanocrystalline Alloys and Magnetic Nanomaterials- Brian Cantor
10. Nanomaterials Handbook- Yury Gogotsi
11. Encyclopedia of Nanotechnology- Hari Singh Nalwa
12. Introduction to Nanotechnology - Charles P. Poole Jr. and Franks. J. Qwens
13. Microwave Properties of Magnetic Films - Carmine Vittoria.
14. Physics of Magnetism - S. Chikazumi and S.H. Charap
15. Physical Theory of Magnetic Domains - C. Kittel
16. Magnetostriction and Magnetomechanical Effects - E.W. Lee
17. Springer Handbook of Nanotechnology - Bharat Bhusan

18. Chemistry of nanomaterials: Synthesis, properties and applications by CNR Rao
19. Synthesis of Nanostructured Materials –Cao
20. Handbook of Nanoscience, Engineering- Goddard et al
21. Nano Engineering in Science & Technology: An introduction to the world of nano design by Michael Rieth.
22. Introduction to Solid State Chemistry – A. R. West
23. Nanocomposites Science and Technology - P. M. Ajayan, L.S. Schadler, P. V. Braun
24. Physical Properties of Carbon Nanotubes- R. Saito
25. Carbon Nanotubes (Carbon , Vol 33) - M. Endo, S. Iijima, M.S. Dresselhaus
26. The search for novel, superhard materials- Stan Vepr¡ek (Review Article) JVST A, 1999.

CHEM 315: EC-II: SOME SELECTED TOPICS IN PHYSICAL CHEMISTRY

Unit-I **COLLOIDAL SCIENCE** **[15L]**

Applied colloids-Surface chemistry and nanocatalysts:

Introduction to the nature of colloidal solution, Surface Tension, Wetting, Solubilisation, Dispersion, Detergency, contact angle measurement, lotus effect, Surfactants and Self-assembly, Emulsions and Micro emulsion, Role of surfactants in synthesis of nanoparticles

Nanocatalysts:

Role of transition metals & metal oxides in homogeneous and heterogeneous catalysis and their mechanism of catalysis, manufacture of these catalysts in nano-form and their characterization.

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

Principles and Concepts of Green Chemistry:

Sustainable development and green chemistry, Atom economy, examples of atom economic and atom un-economic reactions, reducing toxicity.

Waste:

Production, Problems and Prevention: Sources of waste from chemical industry, waste minimization techniques, on-site waste treatment (Physical treatment, Chemical treatment and bio-treatment plants), and design for degradation: Degradation and surfactants, DDT, Polymers, rules for degradation.

Organic solvents:

Environmentally benign solutions: solvent free systems, supercritical fluids-Supercritical carbon dioxide, decaffeination process, $ScCO_2$ as reaction solvent, Supercritical water, ionic liquids as catalysts and solvents.

Unit-III **INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS** **[15L]**

Hyphenated Techniques:

Introduction, need for hyphenation, possible hyphenation, interfacing devices and applications of the following: GC-MS, GC-IR, MS-MS, LC-MS, ICP-MS and Spectro-electrochemistry.

Radio-chemical methods: Auto, X-ray and gamma radiography.

Unit-IV **ADVANCED INSTRUMENTAL TECHNIQUES** **(15L)**

Electron microprobe method, Reflectance spectroscopy, Chemiluminescence method, Photoacoustic spectroscopy,

Polarimetry: ORD, CD.

Reference books:

1. Novel Nanocrystalline Alloys and Magnetic Nanomaterials- Brian Cantor
2. Nanomaterials Handbook- Yury Gogotsi
3. Encyclopedia of Nanotechnology- Hari Singh Nalwa
4. Introduction to Nanotechnology - Charles P. Poole Jr. and Franks. J. Qwens
5. Microwave Properties of Magnetic Films - Carmine Vittoria.
6. Physics of Magnetism - S. Chikazumi and S.H. Charap
7. Physical Theory of Magnetic Domains - C. Kittel
8. Magnetostriction and Magnetomechanical Effects - E.W. Lee
9. Springer Handbook of Nanotechnology - Bharat Bhusan
10. Chemistry of nanomaterials: Synthesis, properties and applications by CNR Rao
11. Synthesis of Nanostructured Materials –Cao
12. Handbook of Nanoscience, Engineering- Goddard et al
13. Nano Engineering in Science & Technology: An introduction to the world of nano design by Michael Rieth.
14. Introduction to Solid State Chemistry – A. R. West
15. Nanocomposites Science and Technology - P. M. Ajayan, L.S. Schadler, P. V. Braun
16. Physical Properties of Carbon Nanotubes- R. Saito
17. Carbon Nanotubes (Carbon , Vol 33) - M. Endo, S. Iijima, M.S. Dresselhaus
18. The search for novel, superhard materials- Stan Vepr¡ek (Review Article) JVST A, 1999.
19. Mike Lancaster, *Green Chemistry: An Introductory Text*, Royal Society of Chemistry, 2002.
20. Paul T. Anastas and John C. Warner, *Green Chemistry – Theory and Practice*, Oxoford University Press, 1998.
21. Albert S. Matlack, *Introduction to Green Chemistry*, Marcel Dekker, Inc., 2001.
22. R.P.W.Scott, *Tandem Techniques*, Wiley India Pvt.Ltd. Reprint 2009.
23. J. Barker, *Analytical chemistry for open learning, Mass spectrometry*, Wiiley IndiaED.
24. H. J. Arnikar, *Essential of Nuclear Chemistry*, New Age International, 1995.
25. G. C. Bond, *Heterogeneous Catalysis*, 2nd ed., Clarendon Press, Oxford, 1987.

SEMESTER-III: INORGANIC CHEMISTRY

Course Code	Title of the Course	No. of Credits	No. of hours per SEMESTER	Examinations		Total Marks
				Continuous Evaluation Marks	End-Sem Marks	
CHEM 321	Solid State Chemistry - I	4	60	40	60	100
CHEM 322	Coordination and Bio-Inorganic Chemistry	4	60	40	60	100
CHEM 323	Instrumental Methods and Spectroscopy	4	60	40	60	100
CHEM 324 EC-II	Advances In Inorganic Chemistry	4	60	40	60	100
CHEM 325 EC-II	Applied Inorganic Materials	4	60	40	60	100
CHEM 326	Inorganic Chemistry Practical III	4	-	-	100	100
CHEM 327	Inorganic Chemistry Practical IV	4	-	-	100	100

No. of CREDITS: 24 TOTAL MARKS: 600

Students will have to select one of the electives i.e. CHEM 324 or CHEM 325

Practical component involves 16 hr per week of laboratory work for 15 weeks.

SEMESTER-III: INORGANIC CHEMISTRY

CHEM 321: SOLID STATE CHEMISTRY-I

Unit-I **[15L]**

(a) Crystal Chemistry:

Structures of the compounds of the types: AB (PbO and CuO), AB_2 (β-crystabalite, CaC_2 and Cs_2O), A_2B_3 (Cr_2O_3 and Bi_2O_3), AB_3 (ReO_3 and Li_3N), ABO_3 (relation between ReO_3 and perovskite, $BaTiO_3$ and its polymorphic forms, oxide bronzes, ilmenite structure), AB_2O_4 (normal and inverse and random spinel structures), Pyrochlores.

(b) Linked polyhedra:

Factors affecting linking of polyhedra, Corner sharing: tetrahedral structure (silicates) and octahedral structure (ReO_3), Edge sharing: tetrahedral structure (SiS_2) and octahedral structures of BiI_3 and $AlCl_3$, etc.

Unit-II **[15L]**

(a) Synthesis of Inorganic Materials: Aspects of inorganic synthesis, choosing a method; Preparation methods: (i) Chemical method (Introduction to ceramic, sol-gel and precursor methods, Topochemical redox reactions,Ion exchange reactions), (ii) High pressure methods, (iii) Arc technique and (iv) Skull melting.

(b) Different methods for single crystal growth:

(i) Crystal growth from solution and flux (Flux growth technique).

(ii) Crystal growth from melt- Bridgman and Stockbargar method, Czochralski technique, Kyropoulos method, Vernuil technique and Zone refining technique.

(iii) Crystal growth from vapor phase: Epitaxial growth methods, chemical vapour transport.

(c) Thin Film Preparation: (i) Chemical and electrochemical methods,

(ii) Physical methods.

Unit-III **[15L]**

(a) Solid Solutions: Formation of substitutional, interstitial and complex solid solutions, mechanistic approach, study of solid solutions by X-ray powder diffraction and by density measurement.

(b) Liquid Crystals: Introduction and classification of different types of liquid crystals, polymorphism in liquid crystals, properties and applications of liquid crystals, inorganic liquid crystals.

Unit-IV[15L]

Crystal defects and non-stoichiometry:

Perfect and imperfect crystals;

Types of defects:

(i) **Point defects**- Vacancy, Self interstitial, Schottky defect, Frenkel defect, thermodynamics of formation of these defects (mathematical derivations to find defect concentration and numerical problems expected), defects in non-stoichiometric compounds: Metal excess defects, Metal deficient defects.

(ii) **Line defects**- Edge dislocation and Screw dislocation

(iii) **Plane defects-** Grain boundaries and Stacking faults

Defect clusters, interchanged atoms; Extended atom defects-crystallographic shear structures, subgrain boundaries and antiphase domains.

CHEM 322: COORDINATION AND BIO-INORGANIC CHEMISTRY

Unit-I INORGANIC PHOTOCHEMISTRY [15L]

Transitions between energy states, decay process, photophysical pathways (fluorescence and phosphorescence), Jablonski diagram, photochemical pathways (unimolecular or intramolecular process and bimolecular or intermolecular process), quantum yield, Kasha's rule and Stoke shifts, identification of excited states, examples of main photochemical processes: non-redox processes (photoisomerization, photodissociation, photosubstitution), photoredox processes: general aspects and mechanism.

Photosynthesis reactions **(**mechanism and salient features of photosynthesis reaction I and II), light harvesting, solar energy conversion, metal ion sensors, chemosensors, artificial photosynthesis.

Unit-II MAGNETIC PROPERTIES OF COMPLEXES [15L]

Origin of magnetism, classification of substances according to the magnetic properties: diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism and ferrimagnetism. magnetic moment from magnetic susceptibility, Curie equation and Curie temperature, Curie-Weiss law, Neel temperature, thermal energy and magnetic moment: multiplet width greater than kT, multiplet width large than kT, temperature independent paramagnetism, magnetic susceptibility and spin only formula, spin and orbital contribution to magnetic moment, spin cross-over.

Magnetic properties of transition metal and lanthanide complexes, magnetic properties of polynuclear and bridged complexes, diamagnetic correction using Pascal constants and calculation of magnetic moment.

Determination of magnetic susceptibility by Gouy, Faraday, Quinke's and NMR methods.

Unit-IIIELECTRONIC SPECTRA OF COMPLEXES

[15L]

Determination of spectral terms for ground state and excited state using pigeon hole diagram, energy of terms, Hund's rules, spin orbit (L-S) coupling , selection rules and intensities, crystal field splitting of the terms in ligand field, construction of Orgel diagram and Tanabe Sugano diagram. Calculation of crystal field parameters (10Dq, B', β, β^o) from electronic absorption spectra of octahedral complexes (d^1-d^9) using Tanabe Sugano diagram, equation method and graphical method (whichever applicable). Comparing the spectra of octahedral, tetrahedral and square planar complexes of Nickel(II). Charge transfer spectra.

Unit-IV BIOINORGANIC CHEMISTRY [15L]

Non-heme iron proteins: Coordination geometry of the metal ion and functions (enzymes with a mononuclear high-spin Fe(II) centre and with mononuclear Fe (III) centre).Zn in biological systems: Carbonic anhydrase, protolytic enzymes, e.g. carboxy peptidase, Zinc finger.Role of metal ions in biological electron transfer processes.Copper containing proteins and enzymes.Less common ions in biology e.g. V, Co, Ni. Metallothionines, Biomineralization.

CHEM- 323: INSTRUMENTAL METHODS & SPECTROSCOPY

Unit-I X-RAY DIFFRACTION [15L]

Introduction to X-ray diffraction, diffraction of waves by crystal, particle and solid, generation of X-rays (K-shell knockout), Bragg condition, Bragg method, Miller indices, relationship between Miller indices and inter planar spacing. Methods of diffraction: Laue method, Debye-Scherrer method of X-ray structural analysis of crystals, advantages of these methods, introduction to JCPDS format, index reflections, identification of Unit- cells from systematic absences in diffraction pattern, uses of powder X-ray diffraction, structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, description of the procedure for an X-ray structure analysis, density and crystallite size determination (numerical problems are expected).

Unit-II [15L]

(a) Electron Diffraction:

Diffraction patterns for single crystal, polycrystalline and amorphous material, difference between X-ray and electron, experimental technique, applications of electron diffraction, low energy electron diffraction, reflection high energy electron diffraction, gas electron diffraction, scattering intensity versus scattering angle and elucidation of structures of simple gas molecules.

(b) Neutron diffraction:

Properties of neutron, principle of neutron scattering, comparison with X-rays, advantages of neutron scattering, scattering of neutron by solids and liquids, experimental technique with essential components, detection of neutrons,

monochromatic technique, time of flight technique, magnetic scattering, applications of neutron scattering.

Unit-III ELECTRON SPIN RESONANCE SPECTROSCOPY [15L]

Introduction, principle, instrumentation, selection rule, relaxation processes and line width in ESR transitions, hyperfine splitting, zero field splitting and Kramer's degeneracy, factors affecting g-value. Calculation of g-values with examples. Intensities of g∥and g ⊥ peaks.

Applications of ESR to the study of simple free radicals and metal complexes like methyl($^{\bullet}CH_3$), cyclopentadienyl ($^{\bullet}C_5H_5$), hydroxyl methyl ($^{\bullet}CH_2OH$), ammonia ($^{\bullet}NH_3$), 1,1-diphenyl-2-picryl hydrazyl (DDPH), pyrazine anion ($C_4N_2^-$), benzene anion ($C_6H_6^-$), bis(salicylaldiminato)copper(II), $IrCl_6^{2-}$, copper acetate dehydrate and [VO(5-chlorosalicylaldehyde-aniline)$_2$].

Unit-IV MOSSBAUER SPECTROSCOPY [15L]

Basic principle, recoil energy and Doppler shift. Instrumentation: sources and absorber; motion devices, detection, reference substances and calibration, isomer shift, temperature shift, quadrupole interaction, magnetic interaction, electronegativity and chemical shift.

Applications:

Iron compounds: low spin and high spin Fe(II) and Fe(III) compounds and complexes, effect of pi-bonding, mono and poly nuclear Iron complexes, spinel oxides and iron-sulphur proteins.

Tin compounds: tin halides and tin oxides, organotin compounds.

Iodine compounds: I_2 and alkali metal iodide compounds.

CHEM 326: INORGANIC CHEMISTRY PRACTICAL-III

I. Separation and estimation of metal ions

1. Separation of Mn and Fe using isoamyl alcohol and estimation of Mn
2. Separation of U and Fe using 8-hydroxyquinoline in chloroform and estimation of U
3. Separation and estimation of Cu(II) and Zn(II) in a mixture using anion exchange resin.
4. Separation and estimation of Ni(II) and Zn(II) in a mixture using anion exchange resin.
5. Separation and estimation of Cu(II) and Ni(II) by forming salicylaldoximinato complexes by varying pH and characterization of complexes using IR.

II. Analysis of the commercial samples

1. Calcium tablet for its calcium content by complexometric titration.
2. Iron tablet for its iron content colorimetry by 1,10-phenonthroline method.
3. Electral powder for Na/K content flame photometrically.
4. Fasting salt for chloride content conductometrically.
5. Cement for its Iron content by redox titration.
6. Washing soda for its Na_2CO_3 content by pH metry.

CHEM 327: INORGAIC CHEMISTRY PRACTICAL-IV

III. Coordination Chemistry

1.Determination of Stability constant of $[Zn(NH_3)_4]^{2+}$ by potentiometry

2.Determination of Stability constant of $[Fe(SCN)]^{2+}$ by slope ratio method

3.Determination of CFSE values of $[Ti(H_2O)_6]^{3+}$ and $[Ni(H_2O)_6]^{2+}$ complexes.

4.Determination of Racah parameters and verification of the spectrochemical series for $[Ni(H_2O)_6]^{2+}$, $[Ni(NH_3)_6]^{2+}$ and $[Ni(en)_3]^{2+}$ complexes.

IV. Synthesis and characterization of Inorganic compounds and materials.

1.Preparation of $VO(acac)_2$ / $[Mn(acac)_3]$ and its characterization by IR, conductivity measurement.

2.Preparation of Hexaamine cobalt (III) chloride and its characterization by IR, and conductivity measurement.

3.Preparation of MnO_2/ZnO/MgO nanoparticles and its characterization by UV-Visible and XRD techniques.

4.Synthesis of bis(salicyl aldiminato)nickel (II) complex / tris(acetyl acetonato)aluminium (III) complex and its characterization using IR and NMR.

5.Synthesis of bis(salicyl aldiminato)copper (II) complex and its characterization by IR and ESR.

6.Synthesis of calcium oxalate/magnesium oxalate and its characterization by TGA/DTA.

7.Synthesis of Prussian blue and its characterization by Mössbauer spectra and cyclic voltammetry.

8.Solid phase synthesis of trans-bis(glycinato)copper(II) and its characterization by IR, and conductivity measurement.

ELECTIVE COURSES

CHEM 324: EC-I: ADVANCES IN INORGANIC CHEMISTRY

Unit-I CHEMISTRY OF GROUP 13 & 14 ELEMENTS

[15L]

Introduction to physical and chemical properties of group 13 and 14 elements. Preparations of various compounds of Al, Ga, In, Tl, Si, Ge, Sn and Pb with special emphasis on hydrides, oxides, halides, sulphides and coordination compounds.

Unit-II

(a) Chemistry of Group 15 and 16 elements: [15L]

Introduction to physical and chemical properties of group 15 and 16 elements. eparations of various compounds of P, As, Sb, Bi, S, Se, and Te, with special emphasis on hydrides, oxides, halides, sulphides, carbides, study of metal nitrides, phosphides, arsenides, antimonides and bismuthides and its applications. Preparation and uses of important compounds like phosphine, azide, hydrazine and hydroxylamine; study of metal sulphides, selenides, tellurides and polonides, ring and cluster compounds, polyanions, polycations and S-N compounds.

(b) Chemistry of Group 17 elements:

Introduction to physical and chemical properties of group 17 elements. reactivity, uses, special properties of fluorine compounds, interhalogens, cationic interhalogens, halogen complex and polyhalides, halogen oxides and fluorocarbons.

Unit-III

[15L]

(a) Preparation of coordination compounds by:

(i) Addition reaction, (ii) Substitution reaction, (iii) Redox reaction, (iv) Thermal dissociation of solid complexes, (v) Reaction in the absence of oxygen, (vi) Reaction of coordinated ligands, (vii) Trans effect.

(b) Steoreochemistry, Chirality and Fluxionality of coordination compoundswith:

Higher coordination numbers, Isomerism and polymorphism in coordination compounds

(c) Crystal Engineering: Metal organic frameworks (MOFs):

Strategies in Coordination Chemistry (Node-and-SpacerApproach), General analysis of Framework Structures (1D, 2D and 3D framework structures), MOFs with Polydentate ligands. Applications of MOFs.

Unit-IV METALLURGY [15L]

Occurrence, extraction and metallurgy of Zirconium, Hafnium, Niobium, Tantalum, Palladium and Platinum. Physical and chemical properties and applications of these metals, compounds of these metals, alloys and their uses.

CHEM-325: EC-II: APPLIED INORGANIC MATERIALS

Unit-I

[15L]

(a) Inorganic Materials:

Classification, manufacture and applications of (i) Inorganic fibers, and (ii) Inorganic fillers. Study of (i) Condensed phosphates, and (ii) Coordination polymers.

(b) Preparation, properties and uses of industrially important chemicals: Sodium peroxide, sodium hydrosulphide, sodium thio sulphate, bleaching powder, hydrogen peroxide, Sodium hydroxide, chlorine and lime.

Unit-II **[15L]**

Supramolecular chemistry:

Definitions, intermolecular bonds, concepts and perspectives, cationic recognition, anionic recognition, neutral molecular recognition: self-assembly concept and its application in molecular and supramolecualar chemistry, supra molecular devices and machines.

Inorganic Pharmaceuticals:

Lithium drugs, gold antiarithritic drugs, bismuth drugs in treatment of gastric ulcers, Cyclams as anti-HIV agents, radio diagnostic agents, contrast agents for X-ray and MRI imaging.

Unit-III MANUFACTURING & APPLICATIONS OF THE FOLLOWING [15L]

(i)Fertilizers and nutrients (ii) Glass (iii) Paints and pigments (iv) Zeolites: synthesis, characterization, determination of surface acidity, shape selectivity, characterizations and applications.

Unit-IV MISCELLANEOUS TOPICS [15L]

(i)Isopoly and heteropoly acids (ii) Intercalation compounds,(iii) Ceramics and refractory materials (iv) Cement (v) Inorganic explosives (lead azide and mercury fulminate).

Reference books:

CHEM-321:

Unit-I:

1. Ulrich Muller, *Inorganic structural chemistry*, 2nd edition, Wiley (2006).
2. A. F. Wells, *Structural inorganic chemistry*, 5th edition, Clarendon press, Oxford (1984).
3. A. R. West, *Solid state chemistry and its chemical applications*, John Wiley & Sons, (1984).

Unit-II:

1. A. R. West, *Solid state chemistry and its chemical applications*, John Wiley & Sons, (1984).
2. Lesley E. Smart and Elaine A. Moore, *Solid state chemistry – An introduction*, 3rd Ed., Taylor and Francis, (2005).
3. C. N. R. Rao and J. Gopalakrishnan, *New directions in solid state chemistry*, Cambridge university press, (1986).

Unit-III:

1. A. R. West, *Solid state chemistry and its chemical applications*, John Wiley & Sons, (1984).
2. C. N. R. Rao and J. Gopalakrishnan, *New directions in solid state chemistry*, Cambridge university press, (1986).

Unit-IV

1. A. R. West, *Solid state chemistry and its chemical applications*, John Wiley & Sons, (1984).
2. H. V. Keer, *Principles of the solid state*, Wiley Eastern Ltd, (1994).

3. Lesley E. Smart and Elaine A. Moore, *Solid state chemistry – An introduction*, 3rd Ed. Taylor and Francis, (2005).

CHEM 322:

Unit-I:

1. J. R. Gispert, *Coordination Chemistry*, Wiley-VCH (2008).
2. D. Banerjea, *Coordination chemistry*, 3rd edition, Asian Books Pvt. Ltd. (2009).
3. R. Gopalan and V. Ramalingam, *Concise coordination chemistry*, Vikas Publising House Pvt. Ltd. (2007).
4. Gary Wulfsberg, *Inorganic chemistry*, Viva Books Pvt,. Ltd. (2002).
5. B. Douglas, D. McDaniel and J. Alexander, *Concepts and models of inorganic chemistry*, 3rd editions, John Wiley & Sons, Inc.(2001).

Unit-II:

1. R. A. Dutta & A. Syamal, *Elements of magnetochemistry*, 2nd edition, Affiliated East-West Press Pvt. Ltd. (1993).
2. D. Banerjea, *Coordination chemistry*, 3rd edition, Asian Books Pvt. Ltd. (2009).
3. R. Gopalan and V. Ramalingam, *Concise coordination chemistry*, Vikas Publising House Pvt. Ltd. (2007).

Unit-III:

1. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic chemistry- Principles of structure and reactivity*, 4th edition, Pearson (2006).
2. A. B. P. Lever, *Inorganic electronic spectroscopy*, Elsevier Publishing Company (1968).
3. R. Gopalan and V. Ramalingam, *Concise coordination chemistry*, Vikas Publising House Pvt. Ltd. (2007).
4. J. E. House, Inorganic chemistry, Academic press, 2nd edition, 2013.

Unit-IV:

1. S. J. Lippard and J. M. Berg, *Principles of bioinorganic chemistry*, University Science Publications, Mill Valley, Caligronic, (1994).
2. R. R. Crichton, *Biological Inorganic Chemistry, A new introduction to molecular structure and function*, 2nd Edition, Elsevier, (2012).
3. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, *Bioinorganic chemistry*, First South Indian Ed., Viva Books, New Delhi, (1998).
4. G. N. Mukherjee and A. Das, *Elements of bioinorganic chemistry*, Dhuri and Sons, Calcutta, (1988).
5. R. W. Hay, *Bioinorganic chemistry*, Ellis Harwood, England, (1984).
6. J. A. Cowan, *Inorganic biochemistry-An introduction*, VCH Publication, (1993).

CHEM 323:

Unit-I-IV:

1. Lesley E. Smart and Elaine A. Moore, *Solid state chemistry – An introduction*, 3rd Ed., Taylor and Francis, (2005).
2. Fmiza Hammer, *Inorganic spectroscopy and related topics*, Sarup & Sons (2008).

3. R. S. Drago, *Physical methods for Chemists*, 2nd edition, Saunders college publishing (1992).
4. R. S. Drago, *Physical methods in Inorganic chemistry*, Affiliated East-West Press Pvt. Ltd; New Delhi.
5. R. A. Scott and C. M. Lukehart, *Applications of physical methods to inorganic and bioinorganic chemistry*, John Wiley & Sons Ltd. (2007).
6. D. N. Sathyanarayana, *Introduction to magnetic resonance spectroscopy ESR, NMR, NQR*, I. K. Intenational publishing house pvt. Ltd. (2009).
7. K. Burger, *Coordination chemistry: Experimental methods*, London Butterworths, (1973).
8. R. V. Parish, *NMR, NQR, EPR and Mossbauer spectroscopy in Inorganic Chemistry, Ellis Horwood.* (1990).

Reference books for practicals

CHEM326:

Unit-I:

1.Gopalan, Universities Press India Pvt.Ltd. *Inorganic Chemistry for Undergraduates*, (2009).
2.P. L. Soni, *Textbook of Inorganic Chemistry*. Sultan Chand & Sons Publisher, 15th Edition (1984).
3.J. D. Lee, 5thEdn.,*Concise Inorganic Chemistry*, ELBS, (2010).
4.M. Weller, T. Overton, J. Rourke and F. Armstrong, *Inorganic chemistry*, 6thedition, Oxford University Press (2015).

Unit-II:

1.M. Weller, T. Overton, J. Rourke and F. Armstrong, *Inorganic chemistry*, 6thedition, Oxford University Press (2015).
2.P. L. Soni, *Textbook of Inorganic Chemistry*. Sultan Chand & Sons Publisher, 15th Edition (1984).
3.J. D. Lee, 5thEdn.,*Concise Inorganic Chemistry*, ELBS, (2010).

Unit-III:

1.S. F. A. Kettle, *Coordination compounds*, Thomas Nelson and Sons Ltd. (1975).
2.D. Banerjea, *Coordination chemistry*, 3rd edition, Asian Books Pvt. Ltd. (2009).
3.R. Gopalan and V. Ramalingam, *Concise coordination chemistry*, Vikas Publising House Pvt. Ltd. (2007).
4.J. R. Gispert, *Coordination Chemistry*, Wiley-VCH (2008).

Unit-IV:

1.R.Gopalan, Universities Press India Pvt.Ltd. *Inorganic Chemistry for Undergraduates*, (2009).
2.P. L. Soni, *Textbook of Inorganic Chemistry*. Sultan Chand & Sons Publisher, 15th Edition (1984).
3.J. D. Lee, 5thEdn.,Concise Inorganic Chemistry, ELBS, (2010).

CHEM 327:

Unit-I:

1.J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic chemistry- Principles of structure and reactivity*, 4th edition, Pearson (2006).
2.P. L. Soni, *Textbook of Inorganic Chemistry*. Sultan Chand & Sons Publisher, 15th Edition (1984).

Unit-II:

1.J. R. Gispert, *Coordination Chemistry*, Wiley-VCH (2008).
2.J. M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, 38 Weinheim, (1995).
3.D. F. Shriver and P. W. Atkins, *Inorganic chemistry*, 3rd edition, Oxford University Press (1999).
4.J. H. Block, E. B. Roche, T. O. Soine and C. O. Wilson, *Inorganic medicinal and pharmaceutical chemistry*, Lea and Febiger, (1974).

Unit-III:

1.P. L. Soni, *Textbook of Inorganic Chemistry*. Sultan Chand & Sons Publisher, 15th Edition (1984).
2.Lesley E. Smart and Elaine A. Moore, *Solid state chemistry – An introduction*, 3rd Ed., Taylor and Francis, (2005).

Unit-IV:

1.J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic chemistry- Principles of structure and reactivity*, 4th edition, Pearson (2006).
2.P. L. Soni, *Textbook of Inorganic Chemistry*. Sultan Chand & Sons Publisher, 15th Edition (1984).

Reference books for practicals:

1. A. I. Vogel, *Quantitative Inorganic Analysis.*
2. J. D. Woolins, *Inorganic Experiments.*
3. Palmer, *Inorganic Preparations.*
4. G. Raj, *Advanced Practical Inorganic Chemistry.*
5. J. E. House, Inorganic chemistry, Academic press, 2nd edition, (2013).

SEMESTER-III: ORGANIC CHEMISTRY

Course Code	Title of the Course	No. of Credits	No. of hours per SEMES-TER	Examination		Total Marks
				Continuous Evaluation Marks	End-Sem Marks	
CHEM 331	Photochemistry, Stereochemistry, Physical Organic Chemistry, and Pericyclic Reactions	4	60	40	60	100
CHEM 332	Ylids, α-C-H Activation And Reactions, Radicals and Organometallic Chemistry	4	60	40	60	100
CHEM 333	Heterocyclic Chemistry and Advanced Spectroscopic Techniques-I	4	60	40	60	100
CHEM 334 EC-I	Medicinal, Green & Bioorganic Chemistry	4	60	40	60	100
CHEM 335 EC-II	Enzymes, Coenzymes & Biogenesis	4	60	40	60	100
CHEM 336	Organic Chemistry Practical III	4	-	-	100	100
CHEM 337	Organic Chemistry Practical IV	4	-	-	100	100

No. of CREDITS: 24 TOTAL MARKS: 600

Students will have to select one of the electives i.e. CHEM 334 or CHEM 335

Practical component involves 16 hr per week of laboratory work for 15 weeks.

SEMESTER-III: ORGANIC CHEMISTRY

CHEM 331: PHOTOCHEMISTRY, STEREOCHEMISTRY, PHYSICAL ORGANIC CHEMISTRY, AND PERICYCLIC REACTIONS

Unit-IPHOTOCHEMISTRY **[15L]**

1.**Photochemistry:**

1.1 **General Principles**-Importance and applications of photochemical processes, Mechanism of absorption of photochemically relevant radiation, Excitation and deactivation of molecules, Electronic transitions and states, Selection rules, notations, types and characteristics, Electron energy transfer,photosensitization and quenching processes. **[3L]**

1.2 Photochemistry of carbonyl compounds, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions, Norrish type-I and Norrish type-II cleavages, Patterno-Buchhi reactions, photoreductions, photochemistry of enones, cyclohexadienones, rearrangements of α, β-unstaurated ketones.**[4L]**

1.3 Photochemistry of unsaturated system-olefins, cis-trans isomerizations and, Di-π methane rearrangement.**[3L]**

1.4 Photochemistry of arenes, 1, 2; 1,3 and 1,4 additions. **[1L]**

1.5 Singlet oxygen and photooxygenation reactions. **[1L]**

1.6 **Intramolecular Rearrangements:** Rearrangements with trimesityl compound to enol ether, o-nitrobenzaldehyde to o-Nitrosobenzoic acid.

Determination of photochemical mechanisms:

1. Use of emission (fluorescence and phosphorescence) and absorption spectroscopy. Energy and life time of singlet and triplet states.

2. The study of quantum yields: primary quantum yields, product quantum yields. **[3L]**

Unit-IISTEREOCHEMISTRY **[15L]**

2.1 Stereochemistry of decalins, hydrindanes, steroids and Bridged ring compounds, Bredt's rule,discussion on non-classical carbocation **[4L]**

2.2 Transannular effects, Addition reactions, elimination reactions **[2L]**

2.3 Classification of point groups based on symmetry elements with appropriate examples [non-mathematical treatment] [**2L]**

2.4 **Molecular dissymmetry and chiroptical properties: [4L]**

Linearly and circularly polarized light, Circular birefringence and Circular dichroism, ORD and CD curves and their applications, The Octant rule and its applications, Applications of CD in conformational studies of biopolymers.

2.5 **Structures, symmetry and synthesis of 3-prismane and cubane: [3L]**

Reactions of cubane and its derivatives, Structures and symmetry of 4/5/6 prismanes and general methods of synthesis of Helicenes and their chiral applications.

Unit-IIIREACTIVE INTERMEDIATES & PHYSICAL ORGANIC CHEMISTRY [15 L]

3.1 **Organic reactive intermediates: [8L]**

Methods of generation, Structure, Stability and important reactions of Carbocations [including NGP and non-classical carbocations], Carbenes, Arynes, Nitrenes, ketenes.

3.2 Acid-base catalysis-General and specific acid and base catalysed reactions, Acidity functions and acidity strength, Reaction rates and acidity scales, Mechanism of acid-base catalysis. **[3L]**

3.3 Potential Energy surfaces, Bell-Evans Polanyi principle, Marcus theory, Curtin-Hammett principle**[2L]**

3.4 **Kinetic methods:**

Determination of reaction order and rate constants, Empirical rate equations for parallel reactions, Sequential reactions. **[2L]**

Unit-IVPERICYCLIC REACTIONS[15L]

4.1 **Role of FMOs in organic reactivity:**

Hard and Soft electrophiles and nucleophiles, Ambident nucleophiles, ambident electrophiles, the α effect.**[3L]**

4.2 **Classification of pericyclic reactions: [1L]**

Thermal and photochemical reactions

4.3 **Three approaches: [2L]**

(1) Conservation of orbital symmetry/Correlation Diagram

(2) Frontier Molecular Orbital approach [FMO] and (3) Aromatic [Huckel and Mobius] Transition state approach.

4.4 **Cycloaddition reactions: [3L]**

4n and (4n+2) π electron systems. Diels-Alder reactions, 1,3-Dipolar cycloadditions and Cheletropic reactions, retro-Diels-Alder reaction. Rates of Diels –Alder reaction based on FMOs; regioselectivity, periselectivity and site selectivity in Diels-Alder reactions.

4.5 **Electrocyclic reactions: [2L]**

Conrotatory and disrotatory motions, 4n and (4n+2) π electron systems and other systems.

4.6 **Sigmatropic rearrangements:[3L]**

H-Shifts and C-shifts, supra and antarafacial migrations. Retention and inversion of configurations. Cope and Claisen rearrangements

4.7 Diimide reduction reactions, *Group transfer reactions **[1L]**

CHEM 332: YLIDS, α-C-H ACTIVATION AND REACTIONS, RADICALS AND ORGANOMETALLIC CHEMISTRY

Unit-IYLIDS, α-C-H ACTIVATION & REACTIONS [15L]

1.1. Methods of preparations, structures and reactivity comparison of phosphorus, sulfur and nitrogen ylides, Reactions of P-, S- and N- ylides with carbonyl compounds and other substrates, including mechanism, stereochemistry and applications in natural product synthesis of Wittig reaction.

1.2. α- C-H activation by nitro, sulfoxide, sulfone and phosphonate groups: generation of carbanions by strong bases (LDA/n-BuLi) and applications in C-C bond formations. Vicarious nucleophilic substitutions.

1.3. Bamford-Stevens Reaction, Julia-Kocienski Olefination, Ramberg-Bäcklund Reaction, Staudinger Reaction, Bestmann-Ohira Reagent, Barton-Kellogg olefination, Steven's rearrangement, Pummerer sulfoxide rearrangement

Unit-IIRADICALS IN ORGANIC SYNTHESIS [15 L]

2.1.**General aspects:**

Electrophilic and nucleophilic radicals and their reactivities with π-rich/deficient olefins.

2.2.Inter- and intramolecular aliphatic C-C bond formation via mercury hydride, tin hydride, carbon hydride, thio donor (Barton's radical decarboxylation reaction).

2.3.Cleavage of C-X, C-Sn, C-Co and C-S bonds in the generation of radicals.

2.4.Trapping by electron transfer reactions using $Mn(OAc)_3$.

2.5.**Radical–Radical processes:**

oxidative couplings, single electron oxidation of Carbanions to generate radicals, dehydrodimerization and Reductive couplings.

2.6.**C-C bond formation in aromatics:**

Introduction, radical reactions on aromatics, electrophilic radical reactions, nucleophilic radicals, Radical reactions on heteroaromatics–alkylations and acylations.

2.7.Hunsdiecker halodecarboxylation, Barton-McCombie alcohol deoxygenation, Kuivila-Beckwith and Stork radical dehalogenation/cyclization, Bergman and Myers-Saito Cycloaromatization.

Unit-IIIMETALS/NON-METALS IN ORGANIC SYNTHESIS [15L]

3.1.Organolithium reagents, Prep and synthetic applications, including directed metallation. Organocupurate reagents.

3.2.Applications of boron: generation of diborane, hydroboration/oxidation of alkenes, alkynes – mechanism, regiochemistry and stereochemistry. Asymmetric hydroboration using chiral borane reagents, functional groups reduction by diborane.

3.3.Mercury in organic synthesis: Oxymercuration-demercuration of alkenes, mechanism and regiochemistry, solvomercuration and intramolecular mercuration. Mercuration of aromatics and transformation of aryl-mercurals to aryl halides.

3.4.Organosilicons: Important features of silicon governing the reactivity of C-Si compounds: Preparation and important C-C bond forming reactions of alkyl silanes, alkenyl silanes, aryl silanes and allyl silanes. Silyl enol ethers as enolate precursors. Iodo trialkyl silane and tralkylsilylcyanide in organic synthesis.

3.5.Organotin compounds: Preparation of alkenyl/aryl and allyl tin compounds and their acylation and Michael reactions.

3.6.Selenium in organic synthesis: preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and seleno-acetals as α-C-H activating groups.

Unit-IV: TRANSITION & RARE-EARTH METALS IN ORGAINC SYNTHESIS [15L]

4.1.Basic concepts, 18 electron rule, oxidative addition, reductive elimination, substitution.

4.2.**Pd and Rh in organic synthesis:**

π-bonding of Pd and Rh with olefins, applications in C-C bond formations including Wacker process, Heck reaction, Negishi coupling reactions, Carbonylation, hydroformylation, decarbonylation, olefin isomerism, aryl amination using Pd reagents. Olefin metathesis (RCM) using catalysis.

4.3.Applications of nickel, cobalt, iron and chromium carbonyls in organic synthesis

4.4.Selected applications of Samarium iodide, and Cerium (IV), in organic synthesis.

4.5.$Eu(OTf)_3$ and $Sc(OTf)_3$ as efficient, water tolerant Lewis acid catalysts in aldol condensation, Micheal reactions, Diels-Alder and aza-Diels-Alder reactions, acylation reactions .

CHEM 333: HETEROCYCLIC CHEMISTRY AND ADVANCED SPECTROSCOPIC TECHNIQUES-I

Unit-IHETEROCYCLIC CHEMISTRY-I [15L]

1.1Introduction, Classification, IUPAC and common names of mono-and bicyclic fused Heteroaromatic compounds. **[5L]**

1.2**Reactivity, important general methods of synthesis and selected applications of the following heterocycles: [10L]**

Pyrazole, imidazole, oxazole, isoxazole, thiazole, benzimidazole, benzoxazole, benzthiazole,pyridine and pyridine N-oxide.

Unit-IIHETEROCYCLIC CHEMISTRY-II [15L]

2.1.Reactivity, important general methods of synthesis and selected applications of the following Heterocycles:

Pyridazine, pyrimidine, pyrazine, oxazine, quinoline, isoquinoline, coumarin, indole, purine, s-triazine, benzodiazepine,piperidine, morpholine.

Unit-IIIADVANCED SPECTROSCOPIC TECHNIQUES-I [15L]

3.1.**FT-IR Spectroscopy:** Principle and applications [**2L]**

3.2.**NMR Spectroscopy:** Relaxation phenomenon and relaxation time, First order, higher order spectra and their simplifications, Double resonance,NOE,NOE difference spectroscopy and chemical shift reagents. **[3L]**

3.3.**Second order spectra:** Spin system notation, AB, AX, AB_2-AX_2, ABX, AMX and A_2B_2-A_2X_2 spin system with suitable examples, Coupling in aromatic and heteroaromatic systems,long range coupling. **[2L]**

3.4.Spectra of diastereotopic systems [**1L]**

3.5.**ESR:** Fundamentals and applications **[2L]**

3.6.**Fluorescence Spectroscopy :** Principles and applications [**2L]**

3.7.**Problems** [**3L]**

Unit-IVADVANCED SPECTROSCOPIC TECHNIQUES-II **[15L]**

4.1.**FT-NMR:**Pulse sequences,pulse widths,spins and magnetisation vectors. **[1L]**

4.2.**^{13}C -NMR:**^{13}C nucleus,^{13}C- chemical shifts,Calculation of ^{13}C- chemical shifts, proton coupled ^{13} C - spectra,^{13}C spectra Integration, proton decoupled ^{13}C- spectra. Off- resonance decoupling,DEPT technique, heteronuclear coupling of carbon to ^{19}F and ^{31}P **[3L]**

4.3.**^{19}F-NMR:** Principles and applications **[2L]**

4.4.**^{31}P- NMR:** Principles and applications **[2L]**

4.5.**Two dimensional NMR:**

Introduction, COSY technique and overview of COSY experiment, how to read COSY spetra, HETCOR technique and overview of the HETCOR experiment, how to read HETCOR spectra. **[2L]**

4.6.NOESY, ROESY, HMBC, INADEQUATE techniques [**2L]**

4.7. Problems **[2L]**

4.8. Applications of NMR in medicine **[1L]**

CHEM 336: ORGANIC CHEMISTRY PRACTICAL-III

Separation and analysis of Ternary mixture: (Minimum 8)

A three component mixture of solids and liquids and belonging to same or different chemical classes. Detection and separation of ternary mixture of same or different physical states (solids and liquids) and same or different chemical classes. [Mixture with same chemical classes separable by physical methods can be given. Identification of all three components with preparation of derivatives for two of the components is expected.

CHEM 337: ORGANIC CHEMISTRY PRACTICAL-IV

One step preparations with column chromatography / steam distillation purification step OR two step preparations: (Minimum 8)

1. 1-Nitronaphthalene from naphthalene [purification by steam distillation].
2. P-Nitrophenol from phenol. [purification by column chromatography].
3. Acetyl ferrocene from ferrocene [purification by column chromatography].
4. M-Nitroaniline from m-dinitrobenzene [purification by column chromatography].
5. Flourenone from flourene [purification by column chromatography].
6. Anthracene-anthraquinone –anthrone

7. Benzoin-benzil-benzillic acid.
8. Acetophenone-acetophenone phenyl hyrazone-2-phenyl indole.
9. 2-Naphthol to 1-phenylazo-2-naphthol to 1-amino-2-naphthol.
10. Cyclohexanone- cyclohexanone oxime-caprolactum
11. Gluocose-1,2,5,6-Di-*O*-diisopropylidine-α-D-glucofuranose

ELECTIVE COURSES

CHEM 334: EC-I: MEDICINAL, GREEN AND BIOORGANIC CHEMISTRY

Unit-I DRUG DISCOVERY/DESIGN & DEVELOPMENT & SYNTHESIS–I [15L]

1.1 **General introduction to discovery of new drugs: [6L]**

Drug discovery without a Lead: Penicillin and Librium.

Lead discovery:

Random screening, non-random (or Targeted) screening

Drug metabolism studies, clinical observations, Rational approach to lead discovery.

1.2 **Lead Modification: Drug design and Development [6L]**

Identification of pharmacophore, functional group modification, structure activity relationship, privileged structures and drug like molecules. Structural modification to increase potency and therapeutic index: Homologation. Chain branching, ring chain transformation, bioisosterism

1.3 **Combinatorial Chemistry: [3L]**

General concepts, split synthesis, peptide libraries, encoding combinatorial libraries.

Unit-II DRUG DISCOVERY/DESIGN & DEVELOPMENT & SYNTHESIS–II [15L]

2.1 Synthesis and application of following drugs: Atorvastatin, Linezolide, Nateglinide, S-omeprazole, Ramipril, Zidovudine (AZT). **[10L]**

2.2. **Steric effect:**

2.3. The Taft and other equations, methods used to correct regression parameters with biological activity.

Hansch analysis: A linear multiple regression analysis **[5L]**

Unit-III GREEN CHEMISTRY & ENZYMATIC PROCESSES [15L]

3.1. **Green Chemistry:**

Introduction, Basic principles of green chemistry with applications. **[3L]**

3.2. **Examples of green synthesis/reaction**

Green Starting materials

Green Reagents

Green Solvents and reaction conditions (Solvent replacement table, Supercritical fluids)

Green Catalysis(Traditional processes and green one)

Synthesis of Ibuprofen, Adipic Acid. **[7L]**

3.2. Enzyme catalyzed Organic Reactions: Hydrolysis, Hydroxylation, Oxidation and Reductions. **[5L]**

Unit-IV BIOORGANIC CHEMISTRY [15L]

4.1. **Nucleic acids: [10L]**

Structure and function of DNA and RNA, genetic code, protein biosynthesis,mutation

4.2.**Recombinant DNA synthesis:** **[5L]**

Phosphodiester, Phosphotriester, Phasphoramidite and H- phosphonate approach including solid phase approach.

CHEM 335: EC-II: ENZYMES, COENZYMES AND BIOGENESIS

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

1.1.Introduction and classification of enzymes.

Properties of enzymes: i) Enzyme efficiency ii) Enzyme specificity. **[5L]**

1.2.**Enzyme Kinetics:**

i) Effect of substrate ii) Other factors affection enzyme kinetics such as temperature, pH etc. **[5L]**

1.3.**Enzymes as Catalyst:**

Specificity of Enzyme Catalyzed Reactions, Rate accelerators. **[5L]**

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

2.1.(i) Mechanism of enzyme action and Synthetic approach of enzyme, Mechanism of alcoholic fermentation.

(ii) Role of main enzymes involved in the synthesis and breakdown of glycogen.

(iii)Glycogen store diseases caused by enzyme deficiency **[7L]**

2.2.Chemical nature of selected enzymes: Co-carboxylase, Coenzyme A, Riboflavin phosphate, UDPG, Glucose-1, 6-diphoaphate. **[6L]**

2.3.Bradford assay for enzyme characterization **[2L]**

Unit-III COENZYMES[15L]

3.1.Chemistry of Coenzymes: structures, mechanism of action and bio-modeling studies of the following coenzymes- thiamine pyrophosphate, lipoic acid, nicotinamide adenine dinucleotide, flavin adenine dinucleotide, pyridoxal phosphate, Vitamin B_{12}. **[12L]**

3.2.Oxygen activation in biological systems with reference to Cytochromes. **[3L]**

Unit-IV BIOGENESIS & BIOSYNTHESES OF NATURAL PRODUCTS **[15L]**

4.1.**Biogenesis:** Precursors, Primary and secondary metabolites, Acetate hypothesis. Mevalonate and Shikimic acid pathways. **[5L]**

4.2.**Biosynthesis:** amino acids, alkaloids, steroids and terpenoids. **[5L]**

4.3.Biosynthesis of selected natural products: L-Tryptophan, Cephaline, Cholesterol, Ephedrine, Citranellal **[5L]**

SEMESTER-III: ANALYTICAL CHEMISTRY

Course Code	Title of the Course	No. of Credits	No. of hours per SEMES-TER	Examination		Total Marks
				Continuous Evaluation Marks	End-Sem Marks	
CHEM 341	Separation Techniques	4	60	40	60	100
CHEM 342	Spectroscopic Techniques	4	60	40	60	100
CHEM 343	Electrochemical Techniques Sensors and Environmental Management	4	60	40	60	100
CHEM 344 EC-II	Special Topics in Analytical Chemistry-I	4	60	40	60	100
CHEM 345 EC-II	Special Topics in Analytical Chemistry-II	4	60	40	60	100
CHEM 346	Analytical Chemistry Practical III	4	-	-	100	100
CHEM 347	Analytical Chemistry Practical IV	4	-	-	100	100

No. of CREDITS: 24 TOTAL MARKS: 600

Students will have to select one of the electives i.e. CHEM 344 or CHEM 345

Practical component involves 16 hr per week of laboratory work for 15 weeks.

SEMESTER-III: ANALYTICAL CHEMISTRY

CHEM 341: SEPARATION TECHNIQUES

Unit-I **[15L]**

1.1 Solvent Extraction: Extraction equilibria of Liquid cation exchangers, liquid anion exchangers and crown ethers. Nature of extracted species. Parameters influencing extraction including e.g. role of diluents, aggregation, third phase formation and counter ion. Applications of liquid-liquid extraction in metallurgy and biotechnology.

Unit-II **[15L]**

2.1 **Supercritical Fluid Extraction:** **[5L]**

Principles, instrumentation and applications.

2.2 Solid Phase Micro Extraction: Sorbents, methodology, applications and automation. **[3L]**

2.3 Ion Exchange Chromatography: Synthetic resin based ion exchangers. Type of resin matrices. Breakthrough volume and capacity. Inorganic ion exchangers, chelating ion exchangers, imprinted functional polymers, ligand exchange for separation of organic molecules and enantiomers. **[7L]**

3.1 **Unit-III** **[15L]**

Ion Chromatography: **[7L]**

Suppressor reactions, instrumentation, standard operating conditions, singlecolumn ion chromatography, coupled ion-chromatography. Applications.

3.2 **Size Exclusion Chromatography:** **[4L]**

Theory, type of packings, molecular mass determination. Large scale purification of large bio molecules.

3.3 **Super Critical Fluid Chromatography:** **[4L]**

Instrumentation, effect of pressure, mobile phases, comparison with LC and GC. Applications.

4.1 **Unit-IV** **[15L]**

Method development in HPLC: **[7L]**

Selection of stationary phases and mobile phases, gradient elution, polarity index, comparison of detectors, hybrid columns, chiral separations and PLRP-S. Concept of Preparative chromatography and UPLC.

4.2 **Membrane based Separations:** **[8L]**

Principles and applications of microfiltration, ultrafiltration, reverse osmosis, dialysis and electrodialysis. Liquid membranes.

Reference books:

1. Solvent Extraction Separation of Elements with Liquid Ion Exchangers, S. M. Khopkar, New Age Science Ltd., (2009).
2. Solvent Extraction Principles and Practice, 2nd Edition, J. Rydberg, M. Cox, C. Musikas, G. Choppin, Marcel Dekker, New York, (2004).
3. Solvent Extraction in Biotechnology, K. Schugert, Springer-Verlag Berlin Heidelberg, New York, (1994).
4. Solvent Extraction Chemistry, T. Sekine, Y. Hasegawa, Marcel Dekker, New York, (1977).
5. Supercritical Fluid Extraction, L. Taylor, WILEY Publishers, New York, (1996).
6. Membrane Separation Process, K. Nath, PHI learning Pvt. Ltd., (2008).
7. Analytical Separation Science (Volume 1-5), J. L. Anderson, A. Berthod, V. Pino, A. M. Stalcup, WILEY-VCH, (2015).
8. Ion Exchange Materials Properties and Applications, 1st Edition, A. A. Zagorodni, Elsevier, (2007).
9. Introduction to Instrumental Analysis, R. D. Brown, McGraw Hill, (1987).
10. Instrumental Methods of Analysis , H. H. Willard, L. L. Meritt, J. A. Dean, Affiliated East-West Press, (1977).
11. Selection of the HPLC Method in Chemical Analysis, S. C. Moldoveanu, V. David, Elsevier, (2017).
12. Principles of Instrumental Analysis, D. A. Skoog, F. James Hollier, T. A. Naiman, Harcourt College Publishers, Harcourt India Pvt. Ltd., (1998).
13. Chemical Separations and Measurements Introduction to Separation Science, B. L. Kauger, L. R. Snyder, C. Howath, John Wiley, New York, (1973).

CHEM- 342: SPECTROSCOPIC TECHNIQUES

Unit-I: **[15]**

1.1 **Infra-Red Spectroscopy:**

Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic **[10L]**

compounds, alcohols, ethers, phenols and amines. Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds), Effect of hydrogen bonding, Solvent effect on vibrational frequencies, Overtones and Combination bands.

1.2 **Raman Spectroscopy:** **[5L]**

Classical and Quantum theory of Raman Scattering, Experimental Methods, Correlation of Infrared and Raman Spectra, Normal Modes of vibrations.

Unit-II: **[15]**

2.1 **Nuclear Magnetic Resonance Spectroscopy (^{1}H-NMR):** **[8L]**

Chemical and magnetic equivalent protons, Chemical shift, Spin-spin coupling, Different types of coupling, Factors affecting to coupling constant, Karplus equation, Spin system (AB, AX, ABX, AMX), Shift reagents, Nuclear Overhouser Effect (NOE).

2.2 **Nuclear Magnetic Resonance Spectroscopy (^{13}C-NMR):** **[7L]**

Introduction, Chemical shift of aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon, Effect of substituents on chemical shift.

Unit-III: **[15]**

3.1 **Mass spectrometry:**

Introduction, Ion analysis, Ion abundance, Factors affecting to the fragmentation, Fragmentation of different functional groups, Molecular ion peak, Isotopic peak, Metastable peak, Nitrogen rule, MacLafferty rearrangement, Retro-Diels-Alder reaction.

Unit-IV: **[15L]**

4.1 **Problems:** **[10L]**

Based on joint applications of IR, ^{1}H NMR, ^{13}C NMR, and Mass spectrometric techniques.

4.2 **Electron Spin Resonance Spectroscopy:**

Introduction, Principle of ESR spectroscopy, Instrumental aspect, the ‘g’ factor, Factors affecting to the ‘g’ value, Hyperfine splitting in various structures, Zero field splitting, Kramers degeneracy, Applications to free radicals and transition metal complexes. **[5L]**

Reference books:

1. Donald Pavia; Gary Lampman, Introduction to Spectroscopy, 4th Edition.
2. Barbara H. Stuart, Infra-red Spectroscopy: Fundamentals and Applications.
3. R. M. Silverstein; F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th Edition, John Wiley and Sons.
4. William Kemp, Organic Spectroscopy

5. Harald Gunther, NMR Spectroscopy, Basic principles, Concepts and Applications in Chemistry.
6. Atta-Ur-Rehman; Verlag; Nuclear Magnetic Resonance: Basic Principles (1986).
7. Phillip Crews; Rodriguez; Jaspars; Organic structure Analysis, Oxford University Press (1998).
8. Joseph B. Lambert; Shurvell; Lightner; Cooks, Organic Structural Spectroscopy, Prentice-Hall (1998).
9. Jackmann and Sternhell S, NMR Spectroscopy of Organic compounds.
10. R. K. Harris, Nuclear magnetic Resonance, Pitman, London, 1983.
11. D. N. Sathyanarayana,Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, I K International Publishing House Pvt. Ltd 2009.
12. Edmond de Hoffmann; Vincent Stroobant, Mass Spectrometry: Principles and Applications, 3rd Edition.

CHEM 343: ELECTROCHEMICAL TECHNIQUES SENSORS AND ENVIRONMENTAL MANAGEMENT

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

1. **Voltammetry and polarography:**

Necessity and development of new voltammetric techniques and their comparison with classical DC polarography, Current sampled (TAST) polarography, Pulse (normal, differential and differential double pulse) Polarography, AC and square wave, linear sweep voltammetry and cyclic voltammetry, criteria of reversibility of electrochemical reactions, Quasi reversible and irreversible processes,

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

2..1 Stripping voltammetry, adsorptive stripping voltammetry, voltammetry with ultra micro electrodes chemically modified electrodes. Applications of electrochemical methods in organic synthesis.

2.2 **Chronotechniques:**

Chronopotentiometry and Chronoamperometry, Chronocoulometry

2.3 **Quartz crystal microbalance:**

Principles, methodology and applications.

Unit-III:

Chemical Sensors: **[15L]**

3.1 **Introduction to principles of chemical sensing:**

Signal transduction, Physico-chemical and biological transducers, Sensor types and technologies. Screen-printed electrodes

3.2 **Physico-chemical sensors and transducers:**

Thermal sensors, Electrochemical sensors (amperometric, potentiometric, conductimetric), Semiconductor transducers (ISFET), Optical transducers (absorption, fluorescence, bio/chemiluminescence, SPR), Piezoelectric and acousticwave transducers, An Overview of Performance and Applications.

3.3 **Biochemical sensors**

Enzymes, Oligonucleotides and Nucleic Acids, Lipids (Langmuir-Blodgett bilayers, Phospholipids, Liposomes), Membrane receptors and transporters, Immunoreceptors.

3.4 **Applications:**

Environmental monitoring, Technological process control, Food quality control, Clinical chemistry, Test-strips for glucose monitoring, Screen printed electrodes, Implantable sensors for long-term monitoring, Forensic science.

Unit-IV:

Environmental Management: **[15L]**

4.1 **Solid waste management:**

Objectives of solid waste management, Hazardous wastes:

Bio-medical, radioactive and E-waste, concept of recycle, reuse and recovery, disposal and management of solid industrial waste, Bioremediation and phytoremediation.

4.2 **Environmental impact assessment:**

Concept, process and evaluation methodology for the same.

Reference Books:

1. Modern Polarographic Methods in Analytical Chemistry, A. M. Bond, Marcel Dekker, New York (1980).
2. Electrochemical Methods, A. J. Bard and L. R. Faulkner, John Wiley, New York (1980).
3. Electrochemistry for Chemists, 2nd Ed., Donald T. Sawyer, A. Sobkowiak and J. L. Roberts, Jr., John Wiley, New York (1994).
4. Cyclic Voltammetry and the frontiers of Electrochemistry, M. Noel and K. I. Vasu, IBH, New Delhi. (1990).
5. Technique and Mechanism in Electrochemistry, P. A. Christensen and A. Hamnett, Blackie Academic and Professional (1994).
6. Electroanalytical Chemistry, Ed. A.J. Bard, Marcel Dekker, New York, A Series of volumes.
7. Electroanalytical Chemistry, J.J. Lingane, 2nd Ed., Interscience, New York (1958).
8. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler, and J.A. Nieman 5th Edition (1998).
9. Jiri Janata, Principles of Chemical Sensors, Plenum Press, 1990
10. Principles of Chemical and Biological Sensors, D. Diamond Editor, John Wiley& Sons, 2000.
11. Chemical Sensors and Biosensors, Brian Eggins, John Willey & Sons, 2002.
12. Sensors, Nanoscience, Biomedical Engineering, and Instruments. Richard Dorf Editor, CRC Taylor & Francis, 2006
13. Optical Biosensors. Present & Future. Editors: F. Ligler, C. Rowe Taitt, Elsevier, 2002.
14. Introduction to Bioanalytical Sensors, Alice Cunningham, John Wiley& Sons, 1998.
15. Chemical Sensors and Biosensors for Medical and Biological Applications, Ursula Spichiger-Keller,Wiley-VCH, 1998.
16. Environmental Chemistry, A.K. De, 2nd Ed., Wiley, 1989.
17. Fundamentals of Environmental Chemistry. S.E. Manahan, 3rd Ed., CRC Press, 2009.

18. Solid and Hazardous Waste Management. S.C. Bhatia, Atlantic Publishers & Distributers (P) Ltd. New Delhi, 2007.
19. Environmental pollution and Control. J. J. Peirce, R. F. Weiner and P. A. Vesilind, 4th Edn. Butterworth-Heinemann, USA, 1998.
20. E-waste: implications, regulations, and management in India and current global best practices. Rakesh Johri, TERI Press, New Delhi, 2009.

CHEM 346: ANALYTICAL CHEMISTRY PRACTICAL III

Organic, medicinal, food, detergents, biochemical, electroanalytical:

Organic analysis:

1. Determination of Sulphur compounds eg. Methyleneblue, crystal violet.

Analysis of medicinal:

2. Complete pharmacopoeial assay of acetyl salicylic acid. (I.P.).
3. Sorensen formol titrations eg. Glycine.
4. Nonaqueous titrations eg. glycine, sodium benzoate, pyridoxine HCl, mebendazole. diazepam tablets, sulphamethoxazole, etc.

Estimation of organic compounds in drug formulations:

5. Benzoic acid and salicylic acid, Aspirin and caffeine, Dextrose and saline injection, Chloramphenicol palmitate suspension, Paracetamol.

Analysis of food products:

6. Iodine value of oils and fats.
7. Fe, Ca, and P in milk powder, Proteins in milk and wheat flour, Lactose in milk by Cole's ferricyanide method.
8. Analysis of alcoholic beverages.

Analysis of detergents:

9. Moisture content, Oxygen releasing compounds, Alkalinity, Tripolyphosphate, Active detergent material (anionic, cationic, non –ionic, ampheteric detergents).

Biochemical analysis: Determination of the following in serum/blood.

10. Uric acid, Sugar, Cholesterol.
11. Analysis of Arsenic from hair by hydride generation technique.

Electroanalytical methods:

12. Determination of mixture of acids eg. HCl and phosphoric acid potentiometrically

using glass electrode.

13. Determination of organic aminesby potentiometric titration in glacial acetic acid.

1. Determination of reversibility of a redox system and area of an electrode by cyclic voltammetry.

CHEM 347: ANALYTICAL CHEMISTRY PRACTICAL IV

Minerals, ores, alloy, spectrometry, water, soil, fertilizer and column Chromatography:

Ores &Alloy:

1. Bauxite:

   Al (gravimeric), Fe (volumetric), Ti (colorimetric).

2. Ilmenite.

   Ti (gravimetric/volumetric), Fe (colorimetric).

3. Steels and stainless steels.

   Ni (homogeneous precipitation), Cr (volumetric), Mn (spectrophotometric).

Spectrophotometry & AAS:

4. Determination of copper and bismuth of a mixture using EDTA spectrophotometrically.
5. Determination of copper by extractive photometry using diethyldithiocarbamate.
6. Determination of tin and zinc in canned food by Atomic Absorption Spectroscopy.
7. **Determination of Water Quality Parameters:**

Soil & fertilizer Analysis:

8. NPK ratio, Determination of micronutrients, Cation exchange capacity.

Column chromatography:

9. Separation of cadmium and zinc on an anion exchanger.
10. Analysis of mixture of alcohols by GC (ethanol, n- propanol, n-butanol, n-pentanol and t-butanol.).
11. Separation and estimation of a mixture of acetophnone, benzene and toluene by HPLC using C_{18} column and acetonitrile + water (60:40) mobile phase.Determination of number of theoretical plates.

ELECTIVE COURSES

CHEM 344: EC-I -SPECIAL TOPICS IN ANALYTICAL CHEMISTRY-I

Unit-I ANALYTICAL BIOCHEMSITRY **[15L]**

1.1 **Body fluids:**

Composition of body fluids and detection of abnormal level of certain constituents leading to diagnosis of diseases.

Physiological and nutritional significances of water and fat soluble vitamins and minerals.

Analyses for constituents of physiological fluids, viz., urine & blood.

Analytical techniques for vitamins

1.2 **Immunological methods:**

General Processes of immune response, Antigen-antibody reactions, Precipitation reactions, radio, enzyme, and fluoro-immuno assays, affinity chromatography.

1.3 **Human nutrition:**

Biological values and estimation of enzymes, carbohydrates, essential amino acids, proteins, and lipids.

Unit-II: CLINICAL CHEMISTRY: (APPLICATIONS OF BIOANALYTICAL APPROACH TO MEDICINES) **[15L]**

2.1 **Biologics:**

Brief introduction of drugs to biologics (pathway)

2.2 **Nuclear medicines:**

Role of radiopharmaceuticals in vivo metabolism of radiopharmaceuticals. Uses and adverse side effects.

Principles of various instruments used for diagnosis of various diseases eg. MRI, CT scan, etc.

Radiopharmaceuticals used in disease treatment (doses regulation) eg. For chemotherapy of cancer.

2.3 **Nanomedicines:**

Importance of nanomedicines: Analytical techniques for quantification of nanoparticles uptake by cells (transmission electron microscopy and flow cytometry).

Bioequivalence of nanomedicines.

Unit-III ANALYTICAL CHEMISTRY IN FORNSIC SCIENCE

General idea **[15L]**

3.1 **Biological:** Analysis of biological stains and materials including blood, semen and saliva (qualitative and quantitative).

3.2 **Analytical toxicology:** isolation, identification and determination of the

following:

Narcotics: Heroin, morphine and cocaine.

Stimulants: amphetamines, cocaine and caffeine.

Depressants: benzodiazepines, Barbiturates and mandrax.

Hallucinogens: LSD and Cannabis.

Metabolites of Drugs in blood and urine of addicts.

Viscera, stomach wash, vomit, and post-mortem blood, for poisons like cyanide, arsenic, mercury, insecticides, and pesticides.

Unit-IV MEMBRANE SCIENCE & TECHNOLOGY **[15]**

4.1 Membranes for saline water treatment

4.2 Ceramic membrane

4.3 Recovery of valuables from waste using liquid membrane methods

4.4 Membrane based separations in chemical and nuclear technology

4.5 Membrane based chemical sensors.

4.6 Track etched membrane.

Reference books:

1. West, E S & Todd, W R, Textbook of Biochemistry,Published by The Macmillan Co, 1956.
2. Parikh's text book of medical Jurisprudence and toxicology, C.K. Parikh, CBS Publishers (1990).
3. Clarke's Isolation and identification of Drugs in Pharmaceuticals, body fluids and post-mortem material, Clarke E.G.C., The Pharmaceutical Press, London.
4. Analytical methods in Forensic chemistry Ed. Math. Ho, Ellis Horwood (1990).
5. Methods of Forensic Science, Ed. F. Landquist, Interscience (1962).
6. High performance liquid chromatography in Forensic Chemistry. E.S. Lurie and J.W. Wittner, Jr, Marcel Dekker N.Y. (1983).
7. Analytical Toxicology Methods Manual Ed. H. Stahr, Iowa State University Press (1977).
8. Official Methods of Analysis of the Association of official Analytical Chemists (AOAC), 14^{TH} Ed. (1984).
9. Linda Fossati Wood, MaryAnn Foote, Targeted regulatory writing techniques: Clinical documents for drugs and biologics.
10. Jeanne Yang: A Pathway to Follow-On Biologics, Hasting Science & Technology Law Journal.
11. Gopal Subramanian, Society of Nuclear Medicine, Radiopharmaceuticals.
12. Harry F. Tibbals, Medical Nanotechnology and Nanomedicine.

CHEM 345: EC-II- SPECIAL TOPICS IN ANALYTICAL CHEMISTRY-II

Unit-I **[15L]**

1.1 **Radiochemical methods:**

Isotope dilution method and activation analysis, radiometric and radio release methods.

Auto, X-ray and gamma radiography.

1.2 **Thermal Methods:**

Simultaneous thermal analysis, Evolved gas analysis: Definition, Instrumentation, Classification of methods (Physical, Chemical and Spectroscopic: mass spectrometry and infrared), Applications.

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

2.1 **Principles and Concepts of Green Chemistr**y:

Sustainable development and green chemistry, Atom economy, examples of atom economic and atom un-economic reactions

2.2 **Waste:**

Production, Problems and Prevention; Sources of waste from chemical industry, on-site waste treatment (Physical treatment and Chemical treatment), design for degradation.

2.3 **Catalysis and Green Chemistry:**

Comparison of catalyst types, Heterogeneous catalysts (zeolites and the bulk chemical industry, catalysts in fine chemicals and pharmaceutical industries, catalytic converters), homogeneous catalysts (transition metal catalysts with phosphene ligands, greener Lewis acids, asymmetric catalysis), phase transfer catalysis, Biocatalysis, Photocatalysis

2.4 **Organic solvents:**

Environmentally benign solutions: solvent free systems, supercritical fluids, ionic liquids as catalysts and solvents.

Unit-III COSMETIC, SOAP & DETERGENT ANALYSIS **[15L]**

3.1 **Cosmetic Analysis:**

Introduction to cosmetics

Hair tonic: 2,5-diaminotoluene, potassium bromate, sodium perborate, pyrogallol, resorcinol, salicylic acid, dithioglycollic acid (in permanent wavers).

Creams and lotions: types of emulsions, chloroform soluble material, glycerol, pH emulsion, ash analysis, non-volatile matter by IR spectroscopy.

3.2 **Soap and Detergents analysis:**

Analysis of soaps and detergents: General scheme of analysis, sampling, alcohol soluble materials, moisture and volatile matter, active ingredient and equivalent combined SO_3^{3-}.

Tests for soaps: total fatty acids, fatty anhydride combined alkali, and anhydrous soap, Unsponified and unsaponifiable matter, Free alkali or free acid, titer test, Iodine value, saponification value, free glycerol.

Tests for synthetic detergents: Unsulfonated or unsulfated matter, ester SO3, Combined alcohols, total combined SO3, Alkalinity, chlorides, silicate, phosphate, borates.

UV spectroscopic analysis of detergents: Biodegradability of detergents, Determination of sodium alkyl benzene sulfonate, determination of sodium toluene sulfonate, determination of sodium xylene sulfonate, determination of germicides in soaps and detergents.

Unit-IV ANALYSIS OF HERBAL BASED PRODUCTS **[15L]**

4.1 **Herbs as a raw material:**

Definition of herb, herbal medicine, herbal medicinal products, herbal drug preparation.

Sources of herbs

Selection, identification and authentication of herbal materials, drying and processing of herbal raw material.

4.2 **Extraction of herbal materials:**

Choice of solvent for extraction

Methods used for extraction and principles involved in extraction.

4.3 **Standardization of herbal formulation and herbal extracts:**

Standardization of herbal extract as per WHO cGMP guidelines.

Physical, chemical, spectral and toxicological standardization, qualitative and quantitative estimations.

4.4 **Various chromatographic techniques for the separation, identification, purification and estimation.**

Reference books:

1. Nuclear and Radiochemistry, 3rd Edition, G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, Wiley, New York, 1981.
2. Nuclear and radiochemistry, K. H. Lieser, 2nd Edition, Weinheim, Germany, Wiley VCH, 2001.
3. Radiochemistry and Nuclear Methods of Analysis, W. D. Ehmann and D. E. Vance, Wiley, New York 1981.
4. Thermal Methods of Analysis, P. J. haines, Blacke, London, 1995.
5. Thermal Analysis, 3rd Edition, W. W. Wendlandt, Wiley, New York, 1985
6. Paul T. Anastas, John C. Werner, Green chemistry: Theory and Practice, Oxford University Press, 1998.
7. Mike Lancaster, Green Chemistry: An Introductory Text, RSC Paperbacks. Chemistry of Natural Products, V. K. Ahluwalia, L. S. Kumar, S. Kumar, Ane Books, India, (2006).
8. High-Performance Thin Layer Chromatography (HPTLC), M. Shrivastav, Springer-Verlag Berlin Heidelberg, New York, (2011).
9. Traditional and Folk Herbal Medicine, Vol. 1, Dr. V. K. Gupta, Daya Publishing House, (2012).
10. A Selection of Prime Ayurvedic Plant drugs-Ancient Modern Concordance, S. Dev, Anamaya Publishers, New Delhi, (2006). F.J. Welcher, Standard methods of chemical analysis, volume 3, part-B, (Soap and Detergents).

SEMESTER-IV: PHYSICAL CHEMISTRY

Course Code	Title of the Course	No. of Credits	No. of hours per SEMESTER	Examination		Total Marks
				Continuous Evaluation Marks	End-Sem Marks	
CHEM 411	Atomic structure, group theory & chemical bonding	4	60	40	60	100
CHEM 412	Electrochemistry-II	4	60	40	60	100
CHEM 413	Physical aspects of polymer, photo-physical & photo-chemical processes	4	60	40	60	100
CHEM 414 OC-I	Intellectual Property Rights & Chemoinformatics	4	60	40	60	100
CHEM 415 OC-II	Research Methodology	4	60	40	60	100
CHEM 416	Research Project	8	*	80	120	200

No. of CREDITS: 24 TOTAL MARKS: 600

Students will have to select one of the optional courses i.e. CHEM 414 OC-I or CHEM 415 OC-II

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

SEMESTER-IV: PHYSICAL CHEMISTRY

CHEM 411: ATOMIC STRUCTURE, GROUP THEORY & CHEMICAL BONDING

Unit-IAPPROXIMATE METHODS [15L]

Variation method (linear and non-linear), Non-degenerate first order perturbation theory, Application to helium atom-ground state, Hückel molecular orbital method: conjugated π systems, Dissociation energy and aromaticity, π-electron densities and bond orders, Theory of electrocyclic reactions –Woodward's-Hoffmann rule, Introduction to extended Hückel molecular orbital method

Unit-II MULTI-ELECTRONIC ATOMS & THEORY OF ANGULAR MOMENTUM [15L]

Anti-symmetry and Pauli principle, Slater determinants, Slater type orbitals, Basis sets, Russell-Saunders coupling, Term symbols, Hund's rules, Normal and anomalous Zeeman effect, Paschen Back effect

Unit-III GROUP THEORY [15L]

Symmetry elements and symmetry operations, Symmetry point groups, Identification of point group of molecules, Representation of groups, Matrix representation of operations, Characters and character tables, Reducible and irreducible representations, Statement of the Great Orthogonality theorem and its consequences, Symmetry adapted linear combination

Unit-IV DIATOMIC & POLYATOMIC MOLEUCLES [15L]

Diatomic molecules:

Born-Oppenheimer approximation, Valence bond theory of hydrogen molecule, Molecular orbital theory of hydrogen molecule ion, Molecular orbitals of homonuclear and heteronuclear diatomic molecules, Bond order, Term symbols.

Polyatomic molecules: Hartee-Fock SCF method and configuration interaction, Walsh diagrams.

Reference books:

1. D. A. McQuarrie and J. D. Simon, *Physical Chemistry - a molecular approach*, Viva Books Private Limited, New Delhi, 1998.
2. D. A. McQuarrie, *Quantum Chemistry*, Viva Books Private Limited, New Delhi, first Indian ed., 2003.
3. R. K. Prasad, *Quantum Chemistry*, 3rd Ed., New Age International Publishers, 2006.
4. Ira N. Levine, *Quantum Chemistry*, 5th Ed., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
5. James E. House, *Fundamentals of Quantum Chemistry*, Second Ed., Academic Press, 2005.
6. Robert L. Carter, *Molecular Symmetry and Group Theory*, John Wiley and Sons (Asia) Pte. Ltd., 2004.
7. T. A. Littlefield and N. Thorley, *Atomic and Nuclear Physics – An Introduction*, Van Nostrand, 1979.

List of Books for further reading:

1. John P. Lowe, *Quantum Chemistry*, 3rd ed., Academic Press, New York, 2006.
2. R. Anantharaman, *Fundamentals of Quantum Chemistry*, McMillan India Limited, 2001.
3. Mahendra R. Awode, *Quantum Chemistry*, S. Chand and Co. Ltd., New Delhi, 2002.
4. David O. Hayward, *Quantum Mechanics for Chemists*, Royal Society for Chemistry, 2002.
5. Jack Simons, *An Introduction to Theoretical Chemistry*, Cambridge University Press, 2003.
6. Victor M. S. Gil, *Orbitals in Chemistry, A Modern Guide to Students*, Cambridge University Press, 2000.
7. A. K. Chandra, *Introduction to Quantum Chemistry*, 4th Ed., Tata-McGraw-Hill, 1994.
8. S. N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books Pvt. Ltd., 1998.
9. R. McWeeny, *Coulson's Valence*, 3rd. Ed., Oxford University Press, 1979.
10. J. N. Murell, S. F. A. Kettle and J. M. Tedder, *The Chemical Bond*, Wiley, 1985.
11. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Ed., John Wiley and Sons (Asia) Pte. Ltd., 1999.
12. D. C. Harris and M. D. Bertolucci, *Symmetry and Spectroscopy*, Oxford University.

CHEM 412: ELECTROCHEMISTRY-II

Principles, Instrumentation and applications of the following:

Unit I **POLAROGRAPHY** **[15L]**

Necessity and development of new voltammetric techniques and their comparison with classical DC polarography, Current sampled (TAST) polarography, Pulse (normal, differential and differential double pulse) Polarography,

Unit II **VOLTAMMETRY**

AC and square wave, linear sweep voltammetry and cyclic voltammetry, criteria of reversibility of electrochemical reactions, Quasi reversible and irreversible processes, stripping voltammetry, adsorptive stripping

voltammetry, voltammetry with ultra-micro electrodes, Chemically modified electrodes, Applications of electrochemical methods in organic synthesis.

Unit III **CHRONOTECHNIQUES & SENSORS** **[15L]**

Electrochemical sensors-potentiometric sensors, amperometric sensors and conductivity measurement; Ion selective field effect transistors -Principle, applications and advantages; Biosensors-Bio catalytic membrane electrodes, enzyme based glucose biosensors; Analysis based on multilayer films-General Principle, film structures; Disposable multilayer pIon systems-General principle, performance and applications; Screen printed electrodes. Quartz Crystal Microbalance: Principles and Applications.

Unit IV **ELECTROPHORESIS** **[15L]**

Zone electrophoresis, factors affecting migration rates, supporting media (gel, paper, cellulose acetate, starch, polyacrylamide, agarose, sephedax, and thin layers).

Techniques of electrophoresis: low and high voltage, SDS-PAGE, isoelectric focusing; continuous and discontinuous electrophoresis, Capillary electrophoresis, electro osmotic flow; Techniques of capillary electrophoresis: zone, gel, isoelectric focusing, isotechophoresis and micellar electrokinetic capillary chromatography, detection and applications.

Reference books:

1. D. A. Skoog, F. J. Holler, and T. A. Nieman, *Principles of Instrumental Analysis*, 5th ed., Philadelphia: Saunders College Publishing, 1998.
2. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 8th ed., Philadelphia: Saunders College Publishing, 2004.
3. A. J. Bard and L. R. Faulkner, *Electrochemical Methods*, Wiley, New York, 1980.
4. A. M. Bond, *Modern Polarographic Methods in Analytical Chemistry*, Marcel Dekker, New York, 1980.
5. J. J. Lingane, Electroanalytical Chemistry, 2nded.
6. A. Braithwaite and F. J. Smith, *Chromatographic Methods*, 5th ed., Kluwer Academic Publisher, 1999.
7. F. W. Fifield and D. Kealey, *5th ed*., Blackwell science Ltd. 2000.
8. Andrew G. Ewing, Ross A. Wallingford, and Teresa M. Olefirowicz, *Analytical Chemistry*, Vol. 61 No. 4.

CHEM 413: PHYSICAL ASPECTS OF POLYMER, PHOTO-PHYSICAL & PHOTO-CHEMICAL PROCESSES

Unit I **POLYMER SCIENCE-I** **[15l]**

Introduction:

Polymer science, Classification of Polymers, Nomenclature of polymers, Isomerism in Polymer chains, History of Polymers, Intermolecular forces in Polymers, Conformations in polymer chains.

Molecular weight of polymers:

Solubility, Average molecular weight values, Fractionation of polydisperse systems, Light scattering, GPC, Collegative molecular weights : Osmometry, End group analysis, Other techniques : Ultracentrifugation, Mass spectrometry, Viscometry.

The Synthesis of Polymers:

Chain growth (Addition) polymerization: Mechanism, and kinetics of free radical, cationic and anionic polymerization, Chain transfer reactions, Mayo equation, Thermodynamic aspects of polymerization

Copolymerization: Kinetics of copolymerization, monomer reactivity ratios, determination of monomer reactivity ratios, The *Q-e* scheme, block copolymers, graft copolymers, dendtires

Unit II **POLYMER SCIENCE-II** **[15L]**

Techniques of polymerization (Phase systems in polymerisation): Bulk polymerization, Solution polymerization, Precipitation polymerization, Suspension polymerization, Emulsion polymerization

Step-growth polymerization (Polycondensation): Molecular weight in a step-growth polymerization, Mechanism of polycondation, Kinetics of polycondation.

Polymer reactions, degradation and additives: Polymer analog reactions and Cross-linking reactions.

Polymer degradation and stability: Thermal degradation, Oxidative and UV stability, Chemical and hydrolytic stability, Radiation effect

Polymer additives: Plasticizers, Stabilizers (Heat & UV), Flame retardants, Colorants, Curing agents and other polymer additives

Polymer solutions: Solubility parameter, Solubility of crystalline and amorphous polymers, Thermodynamics of polymer solutions, Flory-Huggins theory of polymer solutions

Unit III **PHOTOCHEMISTRY-I** **[15L]**

Mechanism of Absorption and Emission processes:

Electric dipole transition, Einstein's treatment of absorption and emission phenomena, Time-dependent Schrodinger equation, Time-dependent perturbation theory, correlation with experimental quantities, Intensity of electronic transitions, rules governing transition between two energy states

Physical Properties of Electronically excited molecules:

Nature of changes on electronic excitation, Electronic, vibrational and rotational energies, potential energy diagram, Frank-Condon principle, Emission spectra, Environmental effect on absorption and emission spectra, properties of excited states, excited state acidity constants, dipole moments and redox properties. Types of transitions, fluorescence emission, e-type and p-type delayed fluorescence, phosphorescence emission.

Unit IV **PHOTOCHEMISTRY-I** **[15L]**

Photo-physical Kinetics:

Photokinetic scheme for determination of quantum yields, Kinetics of self

and collisional quenching and Stern- Volmer equation and deviations from Stern Volmer equation, Concentration dependence of quenching and excimer formation, Quenching by added substances: charge transfer mechanism and energy transfer mechanism.

Photo-chemical reactions:

Types of photo-chemical reactions, Selection rules, Kinetics of Photo-chemical reactions. Photochemical reactions of ketones, olefins conjugated olefins and aromatic compounds. Woodward-Hoffman rule of electro-cyclic reactions.

Applications of Photochemistry:

Importance of photochemistry, mutagenic effect of radiation, photosynthesis, mechanism of vision, photo electrochemistry, prospects of solar energy conversion and storage, organic solar cells.

Reference books:

1. P. Bahadur and N. V. Sastry, *Principles of Polymer Science*, second edition, Narosa Publishing House, 2005.
2. C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York, 2010.
3. Joel R. Fried, *Polymer Science and Technology*, Prentice-Hall of India Pvt. Ltd., 2000.
4. V. R. Gowarikar, H. V. Viswanathan and J. Sreedhar, *Polymer Science*. New Age International Pvt. Ltd., New Delhi, 1990.
5. F. W. Billmeyer Jr., *Text Book of Polymer Science*, 3rd edition, John Wiley and Sons, 1984.
6. K.K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, New Age International Publishers, Revised Edition (2003).
7. C.H.DePuy and O.L.Chapman, *Molecular reactions and photochemistry*, Prentice hall of India PVT.LTD. 1988.

Books for further reading:

1. J. M. G. Cowie, *Polymers: Chemistry and Physics of Modern M*aterials, 2nd ed. (first Indian Reprint 2004), Replika Press Pvt. Ltd.
2. G. S. Misra, *Introductory Polymer Chemistry*, New Age International (P) Limited, Publishers, 1993.
3. L. H. Sperling, *Introduction to Physical Polymer Science*. 2nd Edition, John Wiley and Sons. Inc.
4. Hans- Georg Elias, *An Introduction to polymer Science*, VCH 1997.
5. Charles E. Seymour, Jr., *Seymour/Carraher'sPolymer Chemistry*, 6th ed., Marcel Dekker, Inc., 2003.
6. A. Ravve, Principles of Polymer Science, 2nd ed., Kluwer Academic/Plenum Publishers, New York, 2000.

CHEM 416: RESEARCH PROJECT

SEMESTER-IV: INORGANIC CHEMISTRY

Course Code	Title of the Course	No. of Credits	No. of hours per SEMESTER	Examination		Total Marks
				Continuous Evaluation	End-Sem	
CHEM 421	Solid State Chemistry - II	4	60	40	60	100
CHEM 422	Organometallic Chemistry and Catalysis	4	60	40	60	100
CHEM 423	Instrumental Methods, Spectroscopy & Group Theory	4	60	40	60	100
CHEM 424 OC-I	Intellectual Property Rights & Chemoinformatics	4	60	40	60	100
CHEM 425 OC-II	Research Methodology	4	60	40	60	100
CHEM 426	Research Project	8	*	80	120	200

No. of CREDITS: 24 TOTAL MARKS: 600

Students will have to select one of the optional courses i.e. CHEM 424 OC-I or CHEM 425 OC-II

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

SEMESTER-IV: INORGANIC CHEMISTRY

CHEM 421: SOLID-STATE CHEMISTRY-II

Unit-I ELECTRICAL PROPERTIES OF SOLIDS: [15L]

(i) **Ionic conductivity and solid electrolytes:**

Mechanism of conduction in solid electrolytes, e.g. hopping conduction; fast ion conductors, e.g. silver ion conductors, oxygen ion conductors, sodium ion conductors; applications of solid electrolytes, e.g. electrochemical cells, batteries, sensors, fuel cells. Diffusion in Solids: Fick's laws of diffusion, mechanism, Kirkendall effect, diffusion and ionic conductivity.

(ii) **Electrical Properties:**

Band structures of metals, insulators, semi-conductors and inorganic solids; Applications of semiconductors; Other electrical properties: Thomson, Peltier and Seebeck effects, thermocouples and their applications, Hall effect, dielectric, ferroelectric, piezoelectric and pyroelectric materials and their inter-relationship and applications.

Unit-IIMAGNETIC PROPERTIES OF SOLIDS: [15L]

Behaviour of substances in magnetic field, mechanism of ferromagnetic and antiferromagnetic ordering, superexchange, Hysteresis, Hard and soft magnets, Structures and magnetic properties of metals and alloys, transition metal oxides, spinels, garnets, ilmenites, perovskite and magneto-plumbites, Applications in transformer cores, information storage, magnetic bubble memory devices and as permanent magnets.

Unit-III [15L]

(a)Optical Properties of Solids:

Luminescence and phosphor materials: Configurational coordinate model, Anti-Stokes phosphor, Lasers: Ruby laser, Neodymium laser. Absorption and emission of radiation in semiconductor:light emitting diodes, gallium arsenide laser, blue lasers; optical fibers.

(b)**Thermal properties of solids:**

Introduction, heat capacity and its temperature dependence, thermal expansion of metals, ceramics and polymers, thermal conductivity, mechanism of heat conduction metals, ceramics and polymers; thermal stresses.

Unit-IVADVANCES IN NANOMATERIALS [15L]

Introduction to nanotechnology:

Generalpreparative methods for various nanomaterials, functionalization of nanoparticles for various applications (capping), generic challenges in nanomaterial synthesis.

Some important properties of nanomaterials:

Optical properties of metal and semiconductor nanoparticles, magnetic properties.

Some special nanomaterials:

Carbon nanotubes:

Types, synthesis using various methods, growth mechanism, electronic structure; quantum dots: properties and applications. Aerogels: types of aerogels, properties and applications of aerogels.

Applications of nanomaterials in electronics, energy, automobiles, sports and toys, textile, cosmetics, medicine, space and defense. Environmental aspects of nanotechnology.

CHEM 422: ORGANOMETALLIC CHEMISTRY & CATALYSIS

Unit-I ORGANOMETALLIC CHEMISTRY OF p-BLOCK ELEMENTS[15L]

Organometallics of boron group elements (organoboron, organoaluminium, gallium,indium and thallium organyls). Organometallics of carbon group elements (organogermanium, organotin and organolead compounds).Organometallics of nitrogen group elements (organometallics of arsenic, antimony and bismuth). Organometallics of oxygen group elements (organoselenium and organotellurium).

Unit-II [15L]

(a) Organometallic chemistry of f-block elements:

Neutral binary σ-organyls, agostic interactions, carbene complexes, alkynyl compounds, η^5, η^6, η^7 andη^8 compounds.

(b) Metal-metal bonding and metal atom clusters:

Electron count and structures of clusters, synthesis, reactions, isolobal analogy and structures, Wade's rule (applications to boranes, carboranes and organometallic compounds).

Unit-III [15L]

a) Introduction to catalysis andorganometallics as catalysts in organic reactionsinvolving hydrogen:

hydrogenation, asymmetric hydrogenation,hydrosilyation, hydroboration and hydroamination reactions, disilylation and diboration reactions.

(b) Organometallics as catalysts in organic reactionsinvolving carbon monoxide:

Hydroformylation, carbonylation, Water-Gas shift reaction, Fischer-tropsch, alcohol carbonylation, Wacker process, aminocarbonylation reactions.

Unit-IV [15L]

(a)Organometallics as catalysts in organic reactionsinvolving unsaturated hydrocarbons:

Olefin oligomerization (SHOP process, ethene trimerization, propene dimerization and cyclotrimerization of butadiene), alkene isomerization and alkene/alkyne metathesis (alkene metathesis, alkyne metathesis, alkene-alkyne metathesis).

(b) Organometallics in C-X bond formations reactions:
C-C, C-S, C-N bond formation reactions, Heck, Suzuki, Sonogasira, Stille reactions and Reppe Synthesis.

CHEM 423: INSTRUMENTAL METHODS, SPECTROSCOPY & GROUP THEORY

Unit-I [15L]

Infrared spectroscopy:

Introduction to basic principles, instrumentation, factors affecting the character of vibrations, IR absorption bands of metal - donor atom, effect of complex formations on the IR spectrum of ligands like CO_3^{2-}, SO_4^{2-}, NO_3^-, NO_2^-, NH_3, CN^{1-}, CO, olefins (C=C) and CH_3COO^{1-}. Determination of structures of inorganic molecules.

Raman spectroscopy:

Introduction to basic principles andinstrumentation.Applications of Raman spectroscopy in determination of molecular structures like diatomic molecules, triatomic molecules, structure of complex ions in solutions, nitric acid, sulphuric acid.

Nuclear Magnetic Resonance:

Introduction to basic principles and instrumentation. Spectra of paramagnetic materials: Contact shift, application of contact shift, lanthanide shift reagent. Use of ^{1}H, ^{19}F, ^{31}P, ^{11}B NMR spectra in structural elucidation of inorganic compounds.

Unit-II MICROSCOPY FOR SURFACE CHEMISTRY [15L]

Introduction to surface spectroscopy, microscopy, problems of surface analysis, distinction of surface species, sputter etching and depth profile and chemical imaging. Principle, instrumentation and applications offollowing techniques: ion scattering spectra (ISS), secondary ion mass spectroscopy (SIMS), Auger emission spectroscopy (AES), ESCA, scanning electron microscopy (SEM), atomic force microscopy (AFM) and transmission electron microscopy (TEM).

Unit-III THERMAL& OPTICAL METHODS OF ANALYSIS [15L]

(a) Introduction to principles and instrumentation of thermoanalytical techniques TGA, DTA, DSC, Applications of thermal techniques in materials science and industry, Determination of thermodynamic parameters for the reaction employing thermoanalytical measurements.

(b) Circular dichroism (CD) and optical rotatory dispersion (ORD):

Introduction, principle, instrumentation and applications

Unit-IV APPLICATIONS OF GROUP THEORY[15L]

Introduction to of basic concepts of symmetry, Matrix representation of symmetry operations, reducible and irreducible representations, The great orthogonality theorem,

Construction of character tables for point groups C_{2v}, C_{3v} and D_{2h}, Mulliken's notations for irreducible representations, structure of character tables, determination of symmetry species for translations and rotations, reduction of reducible representations using reduction formula.

Application of group theory to infrared and Raman spectroscopy, Symmetry adapted linear combinations, symmetry aspects of MO theory, sigma- and pi-bonding in AB_4 (tetrahedral and square planar), AB_5 (trigonal bipyramidal) and AB_6 (octahedral) molecule.

Reference books:

CHEM 421:

Unit-I:

1.A. R. West, *Solid state chemistry and its chemical applications*, John Wiley & Sons, (1984).

2.Lesley E. Smart and Elaine A. Moore, *Solid state chemistry – An introduction*, 3rd Ed., Taylor and Francis, (2005).

3.R. C. Ropp Warren, *Solid State Chemistry*, Elsevier Science B.V. (2003).

Unit-II:

1.A. R. West, *Solid state chemistry and its chemical applications*, John Wiley & Sons, (1984).

2.Lesley E. Smart and Elaine A. Moore, *Solid state chemistry – An introduction*, 3rd Ed., Taylor and Francis, (2005).

Unit-III:

1.A. R. West, *Solid state chemistry and its chemical applications*, John Wiley & Sons, (1984).

2.W. D. Callister, Jr., (adapted by R. Balasubramaniam), *Callister's Materials science and engineering*, Wiley-India (2010).

Unit-IV:

1.Sulabha K. Kulkarni, *Nanotechnology: Principles and practices*, Capital publishing company (2007)

2.Lesley E. Smart and Elaine A. Moore, *Solid state chemistry – An introduction*, 3rd Ed., Taylor and Francis, (2005).

3.M. Weller, T. Overton, J. Rourke and F. Armstrong, *Inorganic chemistry*, 6thedition, Oxford University Press (2015).

CHEM 422:

Unit-I-IV:

1.Jahn Hartwig, *Organotransition chemistry-From bonding to catalysis*, University science books, California (2010).

2.Christoph Elschenbroich, *Organometallics*, 3rd edition, Wiley-VCH (2005).

3.R. C. Mehrotra and A. Singh, *Organometallic chemistry- A unified approach*, 2nd edition, New Age International (P) Ltd. (2000).

4.R. H. Crabtree, *The organometallic chemistry of the transition metals*, 5th edition, John Wiley & Sons (2009).

5.D. F. Shriver and P. W. Atkins, *Inorganic chemistry*, 3rd edition, Oxford University Press (1999).

6.Gary O. Spessard and Gary L. Miessler, Organometallic Chemistry,3rdedn., Oxford University Press (2015).

CHEM 423:

Unit-I:

1.R. S. Drago, *Physical methods for Chemists*, 2nd edition, Saunders College publishing (1992).
2.R. S. Drago, *Physical methods in Inorganic chemistry*, Affiliated East-West Press Pvt. Ltd; New Delhi
3.Fmiza Hammer, *Inorganic spectroscopy and related topics*, Sarup & Sons (2008).
4.D. N. Sathyanarayana, *Introduction to magnetic resonance spectroscopy ESR, NMR, NQR*, I. K. Intenational publishing house pvt. Ltd. (2009).
5.K. Burger, *Coordination chemistry: Experimental methods*, London Butterworths, (1973).
6.C. E. Housecroft and A. G. Sharpe, *Inorganic Chemistry*, Pearson Education Ltd. 2nd Edition (2005).

Unit-II:

1.D. A. Skoog and F. J. Holler and T. A. Nieman, *Principles of instrumental analysis*, 5th ed., Harcourt Asia PTE Ltd. (1998).
2.R. A. Scott and C. M. Lukehart, *Applications of physical methods to inorganic and bioinorganic chemistry*, John Wiley & Sons Ltd. (2007).
3.Sulabha K. Kulkarni, *Nanotechnology: Principles and practices*, Capital publishing company (2007).

Unit-III:

1.W. W. Wendlandt, *Thermal analysis*, Interscience (1985).
2.P. D. Garn, *Thermoanalytical methods of investigation*, Academic press, N. Y. (1963).
3.A. Blazek, *Thermal analysis*, Van Norstrand Reinhold Co., London (1973).
4.T. Daniel, *Thermal analysis*, Kogan page Ltd., London (1973).
5.C. J. Keattch and D. Dollimore, *An introduction to thermal analysis*, Heyden, London (1975).
6.M. D. Judd and M. I. Pope, *Differential thermal analysis*, Heydon, London (1977).
7.G. W. H. Hohne, W. F. Hemminger and H. Flammerscheim, *Differential scanning calorimetry-An introduction for practioners*, Springer-verlag, Berlin (1996).
8.K. Burger, *Coordination chemistry: Experimental methods*, London Butterworths, (1973).
9.G. W. H. Hohne, W. F. Hemminger and H. Flammerscheim, *Differential scanning calorimetry-An introduction for practioners*, Springer-verlag, Berlin Heidelberg (2003).
10.R. A. Scott and C. M. Lukehart, *Applications of physical methods to inorganic and bioinorganic chemistry*, John Wiley & Sons Ltd. (2007).
11.D. A. Skoog and F. J. Holler and S. R. Crouch, Instrumental analysis, 5th ed., Harcourt Asia PTE Ltd. (1998).

Unit-IV:

1.Gary Wulfsberg, Inorganic chemistry, Viva Books Pvt. Ltd., (2002).
2.J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic chemistry- Principles of structure and reactivity*, 4th edition, Pearson (2006).

3.D. F. Shriver and P. W. Atkins, *Inorganic chemistry*, 3rd edition, Oxford University Press (1999).
4.R. L. Carter, *Molecular symmetry and group theory*, John Wiley & Sons, New York, (1998).
5.S. F. A. Kettle, *Symmetry and structure-Readable Group Theory for Chemists*, 3rd Ed., John Wiley & Sons, Inc. (200&0.
6.K. V. Reddy, *Symmetry and Spectroscopy of molecules*, New Age International (P) Ltd. 2nd Edition, (2009).
*7.*A. S. Kunju and G. Krishnan, *Group theory and its application in chemistry, PHL Learning Pvt. Ltd., (2010).*
8.F. A. Cotton, *Chemical applications of group theory,* Wiley Eastern Ltd., (1989).

CHEM 426: RESEARCH PROJECT

SEMESTER-IV: ORGANIC CHEMISTRY

Course Code	Title of the Course	No. of Credits	No. of hours per SEMESTER			Total Marks
				Continuous Evaluation Marks	End-Sem Marks	
CHEM 431	Stereochemistry, Asymmetric Synthesis, Pericyclic Reactions, Organic Electronic and Photonic materials	4	60	40	60	100
CHEM 432	Advanced Synthetic Organic chemistry	4	60	40	60	100
CHEM 433	Natural Products Chemistry	4	60	40	60	100
CHEM 434OC-I	Intellectual Property Rights & Chemoinformatics	4	60	40	60	100
CHEM 435OC-II	Research Methodology	4	60	40	60	100
CHEM 436	Research Project	8	*	80	120	200

No. of CREDITS: 24 TOTAL MARKS: 600

Students will have to select one of the optional courses i.e. CHEM 434 OC-I or CHEM 435 OC-II

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

SEMESTER- IV: ORGANIC CHEMISTRY

CHEM 431: STEREOCHEMISTRY, ASYMMETRIC SYNTHESIS, THEORETICALLY FASCINATING MOLECULES, ORGANIC ELECTRONIC AND PHOTONIC MATERIALS

Unit-ISTEREOCHEMISTRY[15L]

1.1.Racemates and methods of resolution of racemates.**[3L]**

1.2.Chemical and Instrumental methods of determining configurations. [**4L]**

1.3.Conformation and reactivity in cyclic compounds with more emphasis on cyclohexane derivatives, Reactions involving steric factors and stereoelectronic factors, Addition reactions, substitution reactions, elimination reactions, rearrangement reactions, I-strain concept.**[4L]**

1.4.Determination of enantiomer and diastereomer composition.

(a) Chiroptical methods and their limitations [Horeau effect]

(b) **Methods based NMR:**

Use of Chiral Derivatising Agents, CDA, Chiral Solvating Agents, CSA, and Chiral Shift Reagents, CSR.;

(c) Chromatographic methods, use of chiral stationary phase (chiral columns)**[4L]**

Unit-II ASYMMETRIC SYNTHESIS[15L] Principles of asymmetric synthesis, Cram's rule, Sharpless epoxidation, asymmetric dihydroxylaion, asymmetric aminohydroxylations, asymmetric Diels-Alder reactions, chiral borane reagents, asymmetric reductions of prochiral carbonyl compounds and olefins. Use of chiral auxiliaries in Diastereoselective reductions. Synthesis of alpha amino acids (Corey's Diastereoselective hydrogenation of cyclic hydrazones); Synthesis of L-DOPA [Knowles's Mosanto process], asymmetric aldol and related reactions.

Use of Chiral BINOLs, BINAPs, and chiral oxazolines and oxazolidines in asymmetric transformations.

Unit-III THEORETICALLY FASCINATING MOLEUCLES[15L] 3.1.Structures, synthesis and properties of cyclophanes, calixarenes, C-60, rotaxanes **[5L]**

3.2.Design, operating photophysical principles, synthesis of selected chemo-and fluorescence based metal ion sensors derived from crown ethers and macrocyclic systems, and chemo- and fluorophore chelators. **[8L]**

3.3.**The Host Guest binding phenomena:**

Assessment by UV/VIS or Flourescence methods; NMR methods. The Benesi-Hildebrand Equation, Stern Volmer relationships **[2L]**

Unit-IV ORGANIC, ELCTERONIC & PHOTONIC MOLECULES[15L]

Organic nonlinear chromophores, Conducting polymers, Dye sensitized organic photovoltaic materials, Organic Magnetic materials, Organic light emitting diodes. General examples of organic conjugated chromophores and polymers, synthesis and various applications.

CHEM 432: ADVANCED SYNTHETIC ORGANIC CHEMISTRY

Unit-I DOMINO REACTION & CLICK CHEMISTRY[15L]

1.1.Multi-component reactions: i) Strecker reaction ii) Hantzsch dihydropyridine synthesis iii) Biginelli condensation iv) Passerni 3- component condensation v) Ugi 4- component condensation iv) Domino Knoevenagel-hetero-Diels-Alder reaction.

1.2.Domino Reactions/Tandem Reaction/Cascade Reactions: Definition and Classification

Cascade processes: concept, examples of cationic, anionic and radical initiated cascade reactions.

1.3.Click Chemistry reactions

Unit-II POLYMER SUPPORTED REAGENTS & ELECTROORGANIC SYNTHESIS[15L]

2.1.Polymer supported reagents for acid base catalysis,

2.3.Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes.

2.4.Cathodic reductions: alkyl halides, aldehydes/ketones, nitro compounds, olefin, arenes, Electrodimerizations.

2.5.Anodic oxidations,: Kolbe type reactions, oxidation of arylalkanes .

Unit-III NON-CLASSICAL METHODS OF ORGANIC SYNTHESIS[15L]

Principles and applications of the following:

3.1.1) Phase transfer catalysis, crown ethers and cryptands, concepts, synthesis and applications 2) Micelles, structures, properties and reactions 3) Ionic liquids 4) cyclodextrin, structure and functions 5) ultrasound in organic synthesis 6) Zeolites, structures, properties and catalysis and 7) Organocatalysis 7) Microwave in organic synthesis 8) Solid phase synthesis

Unit-IV DESIGNING ORGANIC SYNTHESIS[15L]

4.1.**Umpolung:**

Concept of umpolung, generation of acyl anion equivalent-1,3-
dithiane from carbonyl compounds, use of methylthio-methylsulfoxide, via

cyanide ion and cyanohydrin ethers, nitro compounds and metallated vinyl ethers

4.2.**Methodology in organic synthesis:**

Functional group interconversions, general methods of 4 -7 membered ring formation, Disconnection approach and Retrosynthetic analysis, ideas of synthones and retrones, Examples of acyclic saturated and unsaturated systems, monocyclic and bicyclic compounds.

4.3.**Target oriented and methods oriented synthesis**: Strategies and tactics.

4.4.**Protection-deprotection of functional groups:**

carbonyl, hydroxyl, amino, carboxyl, with examples illustrating the applications of each.

CHEM 433: NATURAL PRODUCTS CHEMISTRY

Unit-I NATURAL PRODUCTS CHEMISTRY-I[15L]

1.1.**Steroids:**

Occurrence,structures, classification biological role, important structural and stereochemical features of the following types of steroids- Estrogens, gestrogens, androgens, corticosteroids, sterols, bile acids, calciferol, sapogenins and steroidal alkaloids. **[5L]**

1.2. Synthesis of 16-DPA from cholesterol and plant sapogenin. **[3L]**

1.3. Synthesis of commercially important steroids from 16-DPA.**[4L]**

1.4. Synthesis of cinerolone, Jasmolone,allethrolone,pyrethrolone,exaltone and muscone. **[3L]**

Unit-II NATURAL PRODUCTS CHEMISTRY-II[15L]

2.1.**Insect pheromones:**

Structural features and importance .Synthesis of bombycol, gossyplure, disparlure, brevicomin and grandisol **[5L]**

2.2.**Insect growth regulators:**

General idea,constitution of JH, structures of JH_2 and JH_3 [**2L]**

2.3.**Plant growth regulators**:

Structural features and applications of aryl acetic acids, gibberelic acids, brassinolides and triacontanol, Synthesis of triacontanol. **[2L]**

2.4.**Antibiotics:**

Classification on the basis of activity and structure determination of penicillin-G, Cephalosporin-C and terramycin, Synthesis of penicillin-G,phenoxymethyl penicillin and Semi-synthetic cephalosporins. **[6L]**

Unit-III NATURAL PRODUCTS CHEMISTRY-III[15L]

3.1.Carbohydrates

3.2.**Types of naturally occurring sugars:**

Deoxy sugars,amino sugars, branched sugars. Structure determination of lactose, inositol and amino sugars, Constitution and applications of chitin.**[6L]**

3.3.**Natural pigments: [4L]**

General structural features, occurrence, isolation,biological importance and applications of–carotenoids,anthocyanins,flavones,xanthones,quinones,pterins and porphyrins,
Structure determination and synthesis of β-carotene and ubiquinone.

3.4.**Prostaglandins:[3L]**

Classification, General structure and biological importance.
Structure determination and synthesis of PGE_1 and $PGF_{1\alpha}$

3.5.**Lipids:[2L]**

Structure and role of carbolipids,phospholipids and sphingolipids.

Unit-IV NATURAL PRODUCTS CHEMISTRY-IV[15L]

4.1.**Vitamins: [5L]**

Classification, sources and biological importance, Synthesis of B_1,B_2,B_6,D,E, K and compounds with vitamin-K activity.

4.2.**Multi-step synthesis of natural products: [10L]**

Synthesis of the following natural products with special reference to reagents used, stereochemistry and functional group transformations-Reserpine,Longifoline, Griseofulvin, Estrone, β- Vetivone, 4-Demethoxy daunomycin, caryophyllin, etc.

CHEM 436: RESEARCH PROJECT

SEMESTER-IV: ANALYTICAL CHEMISTRY

Course Code	Title of the Course	No. of Credits	No. of hours per SEMESTER			Total Marks
				Continuous Evaluation	End-Sem	
CHEM 441	Quality in Analytical Chemistry and Inorganic Analysis	4	60	40	60	100
CHEM 442	Advanced Instrumental Techniques and Nanotechnology	4	60	40	60	100
CHEM 443	Analysis Of Ores, Food, Agro /Agriculture	4	60	40	60	100
CHEM 444 OC-I	Intellectual Property Rights & Chemoinformatics	4	60	40	60	100
CHEM 445 OC-II	Research Methodology	4	60	40	60	100
CHEM	Research Project	4	*	80	120	200

446						

No. of CREDITS: 24 TOTAL MARKS: 600

Students will have to select one of the optional courses i.e. CHEM 444 OC-I or CHEM 445 OC-II

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

SEMESTER-IV: ANALYTICAL CHEMISTRY

CHEM 441: QUALITY IN ANALYTICAL CHEMISTRY AND PHARMACEUTICAL ANALYSIS

Unit-I: QUALITY IN ANALYTICAL CHEMISTRY **[15L]**

1.1 **The need for reliable results:**

Social and economic impact of wrong analysis, concept of quality, customer requirement, purpose of analysis.

1.2 **Principle of quality assurance quality control:**

Quality management system, quality assurance and quality control, different standards and their main features, best practice.

1.3 **Sampling:**

Definition, types of samples, sampling plan, sub-sampling, sample registration and storage, acceptance sampling- inspection by attributes.

1.4 **Preparation for analysis:**

Method selection, Sources of methods, Factors to consider in choosing a method, performance criteria for methods to determine analytes by selected techniques, reasons for incorrect analytical results, method validation.

1.5 **Making Measurements:**

Good laboratory practice, calibration of measurement, chemical standards and reference materials, quality control, environment, equipment, chemicals, consumables, maintenance and calibration of equipments.

Unit-II **[15L]**

2.1 **Data treatment:**

Control charts, measurement uncertainty: Definition and evaluation of uncertainty; putting uncertainty to use.

2.2 **Documentation and its management:**

Quality manual, record management and reporting results.

2.3 **Managing quality:**

Management system, Standards available for laboratories, audit, review, responsibilities of laboratory staff for quality.

2.4 **Signals and Noise:**

Signal to noise ratio, sources of noise in instrumental analysis, signal to noise enhancement, hardware devices and software methods for noise reduction.

Unit-III: PHARMACEUTICAL ANALYSIS-I **[15L]**

3.1 General idea regarding pharmaceutical industry, definition and classification of drugs, introduction to pharmaceutical formulations, classification of dosage forms.

3.2 Sources of impurities in pharmaceutical chemicals and raw materials.

3.3 Standardization of finished products and their characteristics, official methods of control, use of pharmacopoeia.

3.4 Analysis of compounds based on functional groups (eg. Aspirin, paracetamol, ascorbic acid, vitamin-A), classical and instrumental methods of drug analysis, proximate assays, assays of enzyme containing substances, biological and microbiological assays and tests.

Unit-IV: PHARMACEUTICAL ANALYSIS-II **[15L]**

4.1 Limit tests, solubility tests, disintegration tests, stability studies, impurity profile of drugs, bioequivalence and bioavailability studies.

4.2 Pharmaceutical legislation: Introduction to drug acts, drug rules (schedules), FDA and ISO standards, ISO 9000 and its requirements, introduction to GMP.

4.3 Introduction to drug development.

Reference books:

1. Quality assurance in Analytical Chemistry, Elizabeth Prichard and Vicki Barwick, LGC, Teddington, UK, 2007.
2. Quality Assurance in Analytical Chemistry W. Funk, V. Dammann, G. Donnevert VCH Weinheim (1995).
3. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler, and J.A. Nieman 5th Edition (1998).
4. Good Laboratory practice, Eds. W.Y. Garner, M.S. Barge and J.P. Ussary, ACS Professional Refernce Book (1992).
5. Quantitative Organic Analysis Via functional groups, 3rd Ed. S. Sigia. John Wiley, N.Y. (1972).
6. Pharmaceutical Drug Analysis (Methodology-Theory-Instrumentation Pharmaceutical assays-Cognate Assays), AshutoshKar, New Age Int. Pvt. Ltd. New Delhi (2010).
7. Indian Pharmacopeia 2010, Vol. I, II, III and Addendum 2012, 6th Ed. The Indian Pharmacopoeia Commission, Ghaziabad, 2010.
8. British Pharmacopeia.
9. Pharmaceutical Analysis, T. Higuchi and E. Brochmann- Hanssen, Interscience (1961).
10. The quantitative analysis of drugs, D.C. Garratt, Chapman and Hall (1964).
11. Pharmaceutical Analysis, A.H. Beckett and J.B. Stenlake, Chapman and Hall.
12. Methods of Drug Analysis, B.F. Granbowshi, Lea and Feniger.

13. Analysis of Drugs and Chemicals, N. Evers, W. Smith and C. Grifin.
14. Hawk's Physiological Chemistry, Mc Graw Hill.

CHEM 442: ADVANCED INSTRUMENTAL TECHNIQUES AND NANOTECHNOLOGY

Unit-I **[15L]**

Principles, instrumentation and applications of following:

1.1 Electron spectroscopy: AUGER & UPS.

1.2 Electron microprobe method.

1.3 Reflectance spectroscopy.

Unit-II **[15L]**

Principles, instrumentation and applications of following:

2.1 **Electron microscopy:**
Scanning electron microscopy, Scanning probe microscopes: The Scanning Tunneling Microscope, Atomic force Microscope.

2.2 Chemiluminescence method.

2.3 Photoacoustic spectroscopy.

2.4 **Polarimetry:** ORD, CD**.**

Unit-III HYPHENATED TECHNIQUES **[15L]**

3.1 Introduction, need for hyphenation, possible hyphenation, Interfacing devices and applications of the following: GC-MS, GC-IR, MS-MS, HPLC-MS, ICP-MS, Spectroelectrochemistry and radio-chromatography.

Unit-IV NANOTECHNOLOGY: ADVANCES IN NANOMATERIALS **[15L]**

4.1 Types of nanomaterials, Classification, General preparative methods for various nanomaterials.

4.2 Some important properties on nanomaterials: optical, magnetic properties, Structural and chemical properties.

4.3 Some special nanomaterials: Carbon nanotubes and quantum dots, Preparation and applications.

4.4 Applications of nanomaterials in electronics, energy, automobiles, sports and toys, textile, cosmetics, medicine, space and defense.

4.5 Analytical techniques for characterization of nanomaterials.

Reference Books:

1. Hofmann**,** Siegfried, Auger- and X-Ray Photoelectron Spectroscopy in Materials Science Springer-Verlag Berlin Heidelberg.
2. S. J. B. Reed, I. M. Romanenko, D. S. Woolum, P. Trocellier, Microprobe Analysis.
3. Kuo, John, Electron Microscopy: Methods and Protocols, Humana Press.
4. Gustav Kortüm,Reflectance Spectroscopy: Principles, Methods, Springer; Softcover reprint of the original 1st ed. 1969 edition (January 1, 1969).

5.John W. Birks Chemiluminescence and Photochemical Reaction Detection in Chromatography,Wiley-VCH; (July 26, 1989)
6.Lihong V. Wang, Photoacoustic Imaging and Spectroscopy, CRC press.
7.Douglas A. Skoog; F. James Holler; Stanley R. Crouch; Principles of Instrumental Analysis6th Edition.
8.Handbook of GC/MS Fundamentals and Applications, H. J. Hubschmann, Wienheim, Germany, Wiley VCH, 2001
9.Modern practice of Gas Chromatography, R. L. Grab and E. F.Berry, 4th Edition, Wiley Interscience, New York, 2004.
10.LC/MS: A Practical User Guide, W. C. McMaster, Hooken, Wiley, New Jersey, 2005.
11.Technologies and Applications of Tandem Mass Spectrometry, K. L. Busch, G. L. Glish and S. A. McLuckey, New York, VCH, 1998.
12.Inductively coupled Mass Spectrometry, A. Montaser (Ed), Wiley VCH, Chinchester, 1998, New York.
13.Nanotechnology: Principles and Practices, J. K. Kulkarni, Capital Publishing Co., 2007

CHEM 443: ANALYSIS OF ORES, FOOD, AGRO /AGRICULTURE

Unit I: Analysis of Minerals, Ores and alloys **[15L]**

1.1 Analytical treatment of minerals and ores: Sampling, analytical treatment, dissolution of ores. Biomining.

1.2 Analyses of ores: bauxite and monazite.

1.3 Analysis of alloys: steel and stainless steel and copper based alloys.

Unit II: Soil and Fertiliser Analysis **[15L]**

2.1 Soil health card scheme. Sampling and preparation of soil samples for analysis, solid texture estimation. pH, electrical conductance, organic carbon, $CaCO_3$ (free lime), cation exchange capacity, gypsum requirements, micro and macro nutrients in soil. Soil miro-organisms and their functions.

2.2 Different types of synthetic fertilizers and introduction to organic fertilizers and their analysis and interaction with different components of soil.

Unit III: Food Quality Concepts **[15L]**

3.1 General idea regarding moisture content, ash, fibre, proteins, carbohydrates, lipids and fats in food analysis.

3.2 Food standards – their importance and limitations. Food preservatives, adulterants and contaminants.

3.3 Analysis-

Additives: flavours and colour.

3.4 Contaminant: heavy metals.

Unit IV: Food Analysis & Pesticide Analysis **[15L])**

4.1 Processing and quality control requirements of milk and milk products (butter, cheese, ice cream), carbonated and alcoholic beverages.

4.2 Analysis of dairy products, oils, fruits and vegetables.

4.3 Pesticide Analysis-

Pesticide formulation– Application test.

4.4 Degradation of different insecticides, fungicides and weedicides in soil.

4.5 Pesticide analysis in water, beverages, food products and soil by GC/HPLC/GC-MS.

Texts/ references:

1. Standard methods of Chemical Analysis, Vol. 2, (Part A& B), 5th ed, F. J. Welcher, Von Nostrand & Robert E. Krieger Publishing Co. New York, (1975).
2. Quantitative Organic Analysis, Part III, 2nd Ed., A. I. Vogel, CBS, (1987).
3. Chemical Analysis of Food and Food Products, H. B. Jacob, Van Nostrand Reinhold, (1958).
4. Association of Official Analytical Chemists.

CHEM 446: RESEARCH PROJECT

OPTIONAL COURSES

OPTIONAL PAPER-I

CHEM 414-OC-I / CHEM 424- OC-I/ CHEM 434- OC-I / CHEM 444-OC-I

INTELLECTUAL PROPERTY RIGHTS & CHEMOINFORMATICS

Unit-I [15L]

Introduction to Intellectual Property: [2L]

Histroical 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 illegeal 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 an 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 Breders 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 Cheminformatcs*. 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.

OPTIONAL PAPER-II
CHEM 415-OC-II / CHEM 425- OC-II / CHEM 435- OC-II / CHEM 445-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 commUnit-ites, 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 Approch:

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 egression 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 SAFTEY & 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*, 2nd 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*, 4th Ed. Chapman Hll, London.
4. Harris, D. C., (2007), *Quantitaive chemical analysis*, 6th 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 safet manual 1.01