# DEPARTMENT OF CHEMISTRY TRIPURA UNIVERSITY SURYAMANINAGAR 799 022 CHOICE BASED CREDIT SYSTEM (REVISED 2020)\*

# Course Curriculum – M. Sc. in Chemistry, Tripura University

Somostor I	Course Code (18 Credits core)	Name of the Courses	Marks	Credits	
Semester –1 (	CHEM 701C	Inorgania Chamiatry I	1	00	04
	CHEM 701C	Inorganic Chemistry I		00	04
		Organic Chemistry-I			
	CHEM 703C	Physical Chemistry-I		00	04
a	CHEM 704C	Chemistry Practical-I	1	50	06
Compulsory Elective (8 credits)			4	00	0.4
	CHEM 704E	Basic Statistics		00	04
	CHEM 705E	Computer Skill II	1	00	04
Semester – II (18 Credits core)					
	CHEM 801C	Inorganic Chemistry-II	1	00	04
	CHEM 802C	Organic Chemistry-II	1	00	04
	CHEM 803C	Physical Chemistry-II	1	00	04
	CHEM 804C	Chemistry Practical-II	1	50	06
Elective					
	CHEM 805E	Bio-inorganic Chemistry	5	0	02
	CHEM 806E	Bio-organic Chemistry	5	0	02
	<b>CHEM 807E</b>	Surface Chemistry	5	0	02
	CHEM 808E	Quantum Chemistry	5	0	02
Semester – III (18 credits core)					
	CHEM 901C	Inorganic Chemistry-III	1	00	04
	CHEM 902C	Organic Chemistry-III	1	00	04
	CHEM 903C	Physical Chemistry-III	1	00	04
	CHEM 904C	Chemistry Practical-III	1	50	06
Elective					
	CHEM 905E	Special topics in chemistry	5	0	02
	CHEM 906E	Chemistry of natural products		0	02
	CHEM 907E	Environmental and green chemis		0	02
	CHEM 908E	Advanced group theory	•	0	02
	CILLIVIOUL	riavaneea group incory		·	02
Semester – IV (18 Credits core)					
	CHEM 1001C	Inorganic Chemistry-IV	1	00	04
	CHEM 1002C	Organic Chemistry-IV	1	00	04
	CHEM 1003C	Physical Chemistry-IV	1	00	04
	CHEM 1004C	Chemistry Project – I	5	0	02
	CHEM 1005C	Chemistry Project – II	1	00	04
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#### **SEMESTER I**

# INORGANIC CHEMISTRY - I PAPER – CHEM 701C

Total Marks: 100 (Theory 70 + Internal Assessment 30) Credit: 04

# **Unit-I - Symmetry and Group Theory:**

12L

Symmetry elements and operations, equivalent symmetry elements and equivalent atoms, point groups with examples, Group of very high symmetry, systematic procedures for symmetry classification of molecules and illustrative examples, molecular symmetry for compounds having coordination number 2 to 9, molecular dissymmetry and optical activity.

Brief representation of theory of groups, matrix representation of groups, reducible and irreducible representation of point groups, definition of classes and character, the "Great Orthogonality Theorem", character tables, concept of character projection operator, normal modes of vibrations, symmetry of normal vibration, selection rules for IR and Raman Transitions.

# **Unit-II – Stereochemistry and Bonding:**

12L

Brief review of the Periodic properties, ionic bonding, electronegativity (Pauling, Mulliken and Allred-Rochow methods); review of VSEPR model and the use of outer d-orbitals.

Valence bond theory,hybridization,  $d\pi$ -p $\pi$  bond; LCAO-MO theory for homo-nuclear diatomic molecules; hetero-nuclear diatomic molecule; polyatomic molecules; orbital symmetry and overlap; molecular shapes in terms of molecular orbitals; Walsh Diagrams, non-covalent interactions.

# Unit III- Spectroscopy -I

**12**I

**Infrared and Raman Spectroscopy:** Brief review of basic principles of IR and Raman spectroscopy; application of vibrational spectroscopy in investigating - Symmetry and shapes of simple AB<sub>2</sub>, AB<sub>3</sub> and AB<sub>4</sub>molecules.Structural elucidation (by IR & Raman spectra) of coordination compounds containing the common ligands such as: NH<sub>3</sub>, H<sub>2</sub>O, OH<sup>-</sup>, NO<sup>3-</sup>, SO<sub>4</sub><sup>2-</sup>, ClO<sub>4</sub><sup>-</sup>, CN<sup>-</sup>,SCN<sup>-</sup>,N<sub>3</sub><sup>-</sup>, H<sup>-</sup>, PR<sub>3</sub>, OPR<sub>3</sub>, halides, dioxygen, -COO<sup>-</sup>.

**Mass Spectroscopy:** Basic principle of mass spectrometry, concept of metastable ions and transition, recognition of the molecular ion peak, Application to metal compounds containing ligand such as carbonyl/ nitrosyl/ alkyl/ cyclopentadienyl and acetyl acetonate; Interpretation of mass spectra for structural characterization; Effect of isotopes on the appearance of mass spectrum.

**Mossbauer spectroscopy:** Principles, isomer shift, quadruple effect of magnetic field, application to iron and tin compounds.

# **Unit IV - Basic Bioinorganic Chemistry:**

12L

Essential elements in biological system inorganic elements in biological systems, basic bioenergetics, Structure and function of biological membranes, active transport of cations across membrane, Crown either complexes of Na and K, Ionophores, Sodium /Potassium pump; Metalloporphyrins, heam proteins –haemoglobin and myoglobin: structure, thermodynamics and kinetics of oxygenation.

#### **Recommended Books:**

- 1. J. E. Huheey, E. A. Keiter, R. L Keiter and O. K. Medhi. Principles of Structure and Reactivity. First impression, Pearson Education 2006.
- 2. F. A. Cotton. Chemical Applications of Group Theory (3<sup>rd</sup>Edn) John-Wiley and Sons.
- 3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry (5<sup>th</sup> edition) John Wiley

- 4. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong, Shriver and Atkins Inorganic Chemistry, Oxford University Press (2006).
- 5. Bioinorganic Chemistry, Asim K. Das, Books& Allied Ltd, 2013.
- 6. R. S. Drago, Physical Methods for Chemists (1992), Saunders College Publishing, Philadelphia.
- 7. K. Nakamoto, Infrared Spectra of Inorganic and coordination compounds, 2<sup>nd</sup>Edn. 1970, Wiley-Interscience, London.
- 8. Inorganic Spectroscopic Methods. Alan. K. Brisdan, Oxford Science Publication(Zeneca) 1997).
- 9. Bioinorganic Chemistry (Bertini, Ivano; Gray, Harry B.; Lippard, Stephen J.; Valentine, JoanSelverstone), University Science Books, CA, 1994.

# ORGANIC CHEMISTRY –I PAPER: CHEM 702C

Total Marks: 100 (Theory 70 + Internal Assessment 30) Credit: 04

#### **Unit I: Organic reaction mechanism**

12L

Structure and reactivity of organic molecules, aromaticity, annulenes; Concept of hard and soft acids and bases, isotope effects for determination of reaction mechanisms, Linear free energy relationship; Hammett equation,  $\sigma$ – $\rho$  relationship, non-classical carbenuim ion (or carbocation), kinetic and thermodynamic control, transition states and intermediates, Hammand principle, Curtin-Hammett principle,. General reaction mechanism, aliphatic substitution reaction, SN1, SN2, mixed SN1 and SN2 and SNi reaction, SET reaction, electrophilic substitution reaction, SE1, SE2, SEi mechanism, electrophilic and nucleophilic aromatic substitution reaction, SNAr, SRN1 mechanism, reactivity, effect of substrate, leaving group and attacking nucleophile, elimination reaction, E1 E2 and E1Cb.

# **Unit II: Stereochemistry**

12L

Chirality and isomerism in organic compounds, interconversion of Fischer, Newman and Sawhorse and Flying-wedge formula, *R-S* nomenclature, conformational analysis of cyclic compounds such as substituted cyclohexanes, fused ring systems (decalins, PHA, PHP), symmetry elements and point groups, axial and planar chirality, axial dissymmetry and centro dissymmetry, atropisomerism, stereochemistry of allenes, biphenyls and spiro compounds. Topicity, allylic strains, alkylketone effects, haloketone rule, methods of asymmetric synthesis, enantio-, and diastereo selective synthesis, determination of enantiomeric and diastereomeric excess, methods of resolution, stereospecific synthesis, effect of conformation on reactivity, optical purity, optical activity in absence of chiral atom.

#### **Unit III: Reactive intermediates -I**

12L

Structure, reactivity and stability of carbocations, carbanions, carbenes and nitrenes; classical and nonclassical carbocations; mechanism of condensation reactions involving enolates- Aldol, cross Aldol, Knoevenagel, Claisen, Perkin, Favorski and Stobbe reactions. Rearrangement reactions involving carbocation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement, Demjenov rearrangement, dienone-phenol rearrangement), carbenes (Wolff & Arndt- Eistert synthesis), cyclopropanation, Simon-Smith reaction, rearrangement involving electron deficient nitrogen (Hoffman, Curtius, Schmidt, Lossen, Beckman), and oxygens (Bayear Villiger oxidation, cumene hydroperoxide), PPA cyclization and Fries rearrangement.

#### **Unit IV: Reactive intermediates - II**

12L

**Arynes:** Generation, structure and stability; Benzyne mechanism for aromatic nucleophilic substitution; Rearrangement and cyclo-addition reactions of arynes, synthetic applications.

**Enamines:** methods of preparation, structure and stability of enamines; selectivity in the synthetic applications.

**Free radicals**: Generation, structure and stability of radicals, radical- initiator, scavenger substitution and addition reactions involving radicals, tributyl tin hydride mediated radical reactions, exo- and endo cyclisation and applications

#### **Recommended text and reference books:**

- 1. F. A. Carey and R. J. Sundberg. Advanced Organic Chemistry. 5<sup>th</sup>Edn. Plenum. Part I, Part II.
- 2. J. March, Organic Chemistry, Structure, Reactions and Mechanisms, 4<sup>th</sup>edn, John Willey
- 3. R.T. Morrison and R.N. Boyd, Organic chemistry, 6<sup>th</sup>edn, Prentice hall of India, New Delhi, 2003.
- 4. Michael B. Smith & Jerry March, Advanced Organic Chemistry Reactions, Mechanisms, and Structure. (2013) Wiley-Interscience.
- 5. D. Nasipuri, Stereochemistry, Conformation and mechanism, 2<sup>nd</sup>Edn. John Wiley
- 6. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill, 2007.
- 7. S. Sengupta Basic Stereochemistry of Organic Moleclules, Book Syndicate Pvt. Ltd. 2<sup>nd</sup> Edn.
- 8. P.S. Kalsi, Stereochemistry, Conformation and Mechanism, 8<sup>th</sup> Edition. New Age Int., 2015.
- 9. T. Laue and A. Plagens, Named OrganicReactions, 2<sup>nd</sup> edition (2005), John Wiley & Sons Ltd.
- 10. Reinhard Bruckner Advanced Organic Chemistry, Reaction Mechanisms (2002). Elsevier
- 11. R O C Norman and J M Coxon, Principles of organic synthesis, 3<sup>rd</sup> Edition, CRC Press.
- 12. A Guidebook to Mechanism in Organic Chemistry, P. A. Sykes, Longman Scientific, 1986.
- 13. T. W. Graham Solomons, Craig B. Fryhle, Scott A. Snyder, Organic Chemistry, John Wiley & Sons Inc. 5<sup>th</sup> Edition.
- 14. W. Carruthers, *Some Modern Methods of Organic Synthesis*, Cambridge University Press (2004)
- 15. H. O. House, Modern Synthetic Reactions, 3<sup>rd</sup> Edition (1992), Benjamin Publishing Co.

# PHYSICAL CHEMISTRY - I PAPER: CHEM 703C

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credit: 04

# **Unit –I: Quantum Mechanics:**

12L

# General Principles of Quantum Mechanics

Introduction; linear operators; Hermitian operators and related theorems; uncertainty principle; postulates; properties of wave functions; Schrodinger equation; separability of Schrodinger equation; equation of motion.

# Application to Simple Systems and Approximation Methods

Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential, tunnelling effect and hydrogen atom. Antisymmetry principle and many-electron wave finctions.

# Chemical Bonding

Born-Oppenheimer approximation (Introduction); valence bond (VB) theory and molecular orbital (MO) theory for diatomic molecules – hydrogen molecule ion, hydrogen molecule; excited states of H<sub>2</sub> – singlet and triplet; non-crossing rule and correlation diagram.

# **Unit -II: Kinetic Theory and Transport Properties of Gases:**

12 L

Derivation of Maxwell's distribution of molecular speed; The general equation for transport, Thermal conductivity of gases, Molecular collisions and mean free path, Viscosity of gases, Diffusion, Introduction to the concept of non-steady state, Numerical problems.

# **Unit -III: Spectroscopy-I**

12 L

Rotational(microwave)spectra, rigid diatomic molecule, Energy expression; Rotational constant. Selection rules. Determination of bond length from observed rotational spectra. Spectral intensity-degeneracy of rotational energy levels and total relative population. The effect of isotopic substitution. Non-rigid rotator (energy expression only). Chemical analysis by microwave spectroscopy. Vibrational (infra-red) spectra: Simple harmonic oscillator model. Corresponding selection rule. Anharmonic oscillator model-Morse function. Selection rules. Fundamental absorption and overtones. Hot bands. P-,Q-,R- branch in IR spectra. IR spectra of linear molecules. Parallel and perpendicular vibrations. Chemical analysis by IR techniques.

**Raman spectroscopy:** Rayleigh scattering and Raman scattering (classical and quantum mechanical consideration). Stokes and Anti-stokes lines. Selection rule. O- and S-branch in Raman spectra. Rotational Raman spectra of homonuclear diatomic molecules. Vibrational Raman Spectra. The rule of mutual exclusion. Structure determination from Raman and IR spectra.

Numerical problems.

#### **Unit -IV: Chemical Kinetics-1:**

12 L

Opposing and consecutive reactions, complex reactions, Atomic and free radical chain reactions. Kinetic salt effect; Effect of solvent on rate constant (Single sphere and double sphere model): Non-Arrhenius equations and its significance. Theory of absolute reaction, rate (statistical) and comparison with that of collision theory; Kinetics of enzyme reaction (effect of pH) Michaels- Menton Law, derivation; Numerical problems

# **Suggested reading:**

- 1. G.W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
- 2. D.A.MacQuarrie, *Quantum Chemistry*, (1983) Oxford University press,
- 3. A.K.Chandra, *Introductory Quantum Chemistry*, 4<sup>th</sup> Edition, Tata McGraw Hill, 1997.
- 4. Levine, Quantum Chemistry, (1994)Tata McGraw Hill, New Delhi.
- 5. L. Pauling and E.B.Wilson, *Introduction to Quantum Mechanics with Applications to Chemistry*, (1935), McGraw Hill, New York.
- 6. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3<sup>rd</sup> Ed.(1997) Oxford University Press.
- 7. D. A. McQuarrie and J.D. Simon, *Physical Chemistry*, VIVA Students Ed. (2003)
- 8. J. D. Graybeat. *Molecular Spectroscopy*, McGraw-Hill International Edition
- 9. C. N. Banwell, E. M. McKash; Fundamentals of Molecular Spectroscopy, Tata McGraw Hill.
- 10. K.J.Laidler, Chemical Kinetics, 3<sup>rd</sup> Ed.(1967), Harper and Row Publishers, New York.
- 11. H.Eyring, S.H. Lin and S.M.Lin, *Chemical Kinetics*, (1999)Jhon Willey, New York.
- 12. G. L. Agarwal; Basic Chemical Kinetics, Tata McGraw-Hill.

#### LABORATORY COURSE-I

# PAPER: CHEM 704C (Inorganic Chemistry)

**Total Marks: 100 (Practical 105 + Internal Assessment 45)** 

Credit: 06

- 1. Semi micro qualitative analysis of Inorganic salt mixtures containing (06) six radicals including W, Mo, V, Ti, U, Th, Zr, Ce and at least one interfering radical (F<sup>-</sup>/PO<sub>4</sub><sup>3-</sup>/BO<sub>3</sub><sup>3-</sup>, CrO<sub>4</sub><sup>2-</sup>).
- 2. Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of constituents in three component mixtures and alloys.
- 3. Preparation of the following inorganic compounds and characterization by IR, UV-Visible, Conductance & magnetic susceptibility measurements.
  - (a) Tris (acetyl acetonato)manganese (III)
  - (b)Tris (acetyl acetonato)iron (III)
  - (c) Bis (acetylacetanato) oxovanadium(IV)
  - (d) Renkei's Salt
  - (e)Linkage isomer of nitro &nitridopentammine Cobalt (III) Chloride
  - (f)Tris (Ethylenediammine) Nickel (II) Chloride. Dehydrate

# **Suggested Books**

- 1. J. Mendham, R. C. Danney, J. D. Barnes & M. Thomas. Vogel's Textbook of Quanti-tative Chemical Analysis, Peterson Education (2000).
- 2. G. Marr& B. W. Rockett. Practical Inorganic Chemistry, Van Nostrand (1972).
- 3. G. Pass& H. Sutcliffe. Practical Inorganic Chemistry (2nd edn.), Chapman & Hill (1974)
- 4. G. Brauer, Ed., Handbook of preparative Inorganic Chemistry, Academic Press, Vol 2, 1965,

# **Compulsory Electives**

# BASIC SATISTICS PAPER – CHEM 704E

**Total Marks: 100 (Theory 70 + Internal Assessment 30)** 

Credit: 04

**Syllabus: to be provided by Dean office/Department of Statistics** 

# COMPUTER SKILL II PAPER – CHEM 705E

**Total Marks: 100 (Theory 70 + Internal Assessment 30)** 

Credit: 04

Applications of Computer. Binary Number System: Conversion of binary number into decimal form, Conversion of decimal number into binary form, addition of two binary numbers, multiplication and division, Subtraction of two binary numbers using two's complement. Octal number system: Conversion of octal number into decimal form, Conversion of decimal number into octal form, Conversion of binary number into octal form, Conversion of octal into binary form, Hexadecimal number system: Conversion of Hexadecimal number into binary form, Conversion of binary number into hexadecimal form, Conversion of hexadecimal number into decimal form. Basics of algorithms and Flow chart: Key features of Algorithms: Sequence, decision and repetition. Flowcharts: significance of flowcharts, advantages and limitations. Basics of Programming language Introduction to C: Keywords, identifiers, variables, constants, input/output statement in C, operators in C, decision control and looping statements, arrays and strings. Computation with spreadsheet: Data management using excel-sorting, filtering, validation, Basic functions, logical functions, mean, mode, median, standard deviation, correlation, Chart

#### SEMESTER II

# INORGANIC CHEMISTRY - II PAPER – CHEM 801C

Total Marks: 100 (Theory 70 + Internal Assessment 30) Credit: 04

# **Unit I – Spectroscopy-II:**

12L

**Nuclear Magnetic Resonance Spectroscopy -** Basic principle, Relaxation time-spin lattice and spin–spin relaxation, Chemical shift, factors that affect chemical shift. Use of chemical shifts and spin-spin couplings for structural determination. Application of <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F, <sup>31</sup>P and <sup>119</sup>Sn in the structural assignment of selected inorganic compounds.

**Electron Spin Resonance Spectroscopy** - Electron Paramagnetic Resonance Spectroscopy: Principle, instrumentation, representation of EPR spectrum, X-band and Q-band spectra, line width, hyperfine splitting, magnetically equivalent and nonequivalent sets of nuclei, g-anisotropy, spectra of simple organic free radicals: expected number of lines, intensities. Spectra of transition metal complexes( $d^1$ - $d^9$  ions in cubic and tetrahedral fields), metal hyperfine anisotropic spectra, zerofield splitting, Kramers degeneracy, application: determination of oxidation state of metal ion in samples

# **Unit II - Magneto-chemistry:**

12L

Different types of magnetic behaviour of materials and their origin, magnetic susceptibility and magnetic moment, measurement of magnetic susceptibility (Gouy and Faraday methods), Derivation of Curie equation for magnetic moment, Curie and Curie-Weiss law, quenching of orbital moments, Magnetic behavior of multi-electron system, orbital coupling, spin-coupling, spin-orbit coupling (RusselSaunder's coupling), spin-orbit coupling constant, j-j coupling, micro-states and term symbols, Lande interval rule, Thermal energy and magnetic moment, anti-ferromagnetism and its exchanged pathways.

# **Unit III -Coordination Chemistry:**

12L

Brief review of theories of coordination compounds (VBT, CFT), Ligand Field Theory (LFT), Electronic absorption spectra of octahedral and tetrahedral complexes, Orgel diagrams, Tanabe- Sugano diagrams, calculation of Dq, B and  $\beta$  values, selection rules, band intensities and band widths, spectra of high spin octahedral and tetrahedral complexes of d<sup>1</sup> to d<sup>9</sup> systems, Spectrochemical series; Adjusted crystal field theory, Nephelauxetic series, Tetragonal distortion, Jahn-Teller effect, Molecular orbital theory of complexes (including complexes with and without  $\pi$  bonding), MO diagrams for octahedral and tetrahedral complexes, Charge-transfer spectra.

# **Unit IV - Analytical Chemistry:**

12L

**Thermoanalytical methods -** Thermo gravimetric analysis, differential thermal analysis and differential scanning calorimetry.

**Electrochemical methods -** Coulometry, Polarography, cyclic voltammetry, electrogravimetry.

**Atomic Emission-Absorption Spectroscopy**- Flame Atomic Absorption Spectroscopy: Principles of atomic absorption spectroscopy, Radiation sources, Flame and electrothermal atomization, Quantitative Analysis, Flame Atomic Emission Spectroscopy: Atomic emission, Principles of flame emission photometry, , Qualitative Analysis, Quantitative Analysis.

# **Suggested reading:**

- 1. Inorganic Chemistry-Principles of Structure and Reactivity, 5th Edn. J. Huhee, E.A. Keiter, R.L.Keiter& O.K. Medhi Pearson Education, New Delhi.
- 2. Shriver & Atkins Inorganic Chemistry, Atkins, Overton, Rourke, Weller, Armstrong, South Asia Edn. 5th Edn. Oxford University Press, 2010.
- 3. R. L. Dutta and A. Syamal, Elements of Magnetochemistry (2ndEdn), EWP (2010)
- 4. J. D. Lee, Concise Inorganic Chemistry (5thEdn) John Wiley & Sons (1996).
- 5. R.S. Drago, Physical Methods for Chemists(1992), Saunders College Publishing, Philadelphia.
- 6. J. A. Iggo, NMR Spectroscopy in Inorganic Chemistry, OUP Oxford (2000)
- 7. Fundamental Concepts of Inorganic Chemistry, Vol.7, Asim.K.Das & Mahua Das, CBS Publishers & Distributors, Pvt. Ltd., New Delhi, 2014.
- 8. Inorganic Spectroscopic Methods. Alan. K. Brisdan, Oxford Science Publication(Zeneca) 1997).
- 9. Basic Concepts of Analytical Chemistry, S.M. Khopkar, New Age international Ltd, Publishers, New Delhi.\
- 10. A Text-book of Quantitative Inorganic Analysis including Elementary Instrumental Analysis, by A.I. Vogel, 3<sup>rd</sup> Edition, The English language book Society and Longmans, Green & Co Limited, (1956).

# ORGANIC CHEMISTRY –II PAPER: CHEM 802C al Marks: 100 (Theory 70 + Internal Asse

Total Marks: 100 (Theory 70 + Internal Assessment 30) Credit: 04

# Unit I: Strategies and reagents in organic synthesis

12L

Designing of organic synthesis - Retrosynthetic and Disconnection approach; Reversal of dipoles (umpolung of reactivity) and it's applications; Synthons and retrons, linear and convergent synthesis, protection and deprotection strategies for common functional groups in organic synthesis; Applications of crown ether and phase transfer catalyst. Uses of the following reagents in organic synthesis: IBX, Dess-Martin periodinane, chloranil, DDQ, K-selecteride and L-selecteride, sodium cyanoborohydride, super hydrides, 9-BBN, Mukaiyama reagent, LDA, dicyclohexylcarbodimide, Corey-Nicolaou reagent, baker's yeast, CBS reagents.

# Unit -II: Unit II: Orbital symmetry reaction

12L

Orbital symmetry, electrocyclic, cycloaddition, sigmatropic and group transfer reactions; Woodward-Hoffmann rule in pericyclic reactions; Rationalization based on FMO approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems. Chelatropic reactions, 1,3-dipolar cycloaddition Cope, aza-Cope, oxy-Cope, Claisen, Somelett-Hauser rearrangements.

**Photochemistry:** Cis-trans isomerisation, Paterno-Buchi reaction, Norrish type I & II reaction, photoreduction of Ketones, di-pi-methane rearrangement, photochemistry of arenes, Photo-Fries rearrangement of ethers and anilides; Hoffmann-Loefller-Freytag Reaction, Barton reaction.

# **Unit III: Oxidation and reduction reactions of organic compounds:**

12L

**Oxidation:** Oxidation by Cr and Mn compounds; oxidation of alcohol, aldehyde, C=C, C-H bonds, PCC, oxidation with per acids and peroxides, ceric ammonium nitrate, Thallium(III) nitrate, Prevost and Woodward hydroxylation, cis- and trans- hydroxylation, glycol cleavage reagents: KMnO<sub>4</sub>, OsO<sub>4</sub>, HIO<sub>4</sub>, Pb(OAc)<sub>4</sub>, mercuric acetate, SeO<sub>2</sub> oxidation of allylic C-H bond. Epoxidation of alkenes- Sharpless epoxidation.

**Reduction:** Catalytic hydrogenation and dehydrogenation, dissolving metal reduction, reduction of functional groups, Meerwein-Pondrof-Verley reduction, hydroboration and related reaction, reaction of alkyl borane, Wolff-Kishner reduction, non-metallic reducing agents such as diimide.

#### **Unit IV: Selective named reactions**

12L

Swern oxidation, Moffat oxidation, Henry reaction, Wittig reaction and Horner-Wordwoth-Emmons reaction (stabilized and non-stabilized ylide); Nazarov cyclization, Pictet-Sprengler reaction, Passerini reaction, Ugi reaction, Peterson's synthesis, McMurry olefination, Julia olefination, Shapiro reaction, Chichibabin reaction, Baylis-Hillman Reaction, Staudinger Reaction.

# **Suggested reading:**

- 1. R O C Norman and J M Coxon, Principles of organic synthesis, 3<sup>rd</sup> Edition, CRC Press.
- 2. A Guidebook to Mechanism in Organic Chemistry, P. A. Sykes, Longman Scientific, 1986.
- 3. T. W. Graham Solomons, Craig B. Fryhle, Scott A. Snyder, Organic Chemistry, John Wiley & Sons Inc.
- 4. W. Carruthers, Some Modern Methods of Organic Synthesis, Cambridge University Press
- 5. T. Laue and A. Plagens, Named Organic Reactions, 2<sup>nd</sup> edition (2005), John Wiley & Sons Ltd.
- 6. H. O. House, Modern Synthetic Reactions, 3<sup>rd</sup> Edition (1992), Benjamin Publishing Co.
- 7. S. Warren, Organic Synthesis, Disconnection Approach, 1982, Wiley Interscience, NY
- 8. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry Part A and Part B.
- 9. T. Laue and A. Plagens, Named Organic Reactions, 2<sup>nd</sup> edition (2005), John Wiley & Sons Ltd
- 10. J. March, Organic Chemistry, Structure, Reactions and Mechanisms, 4<sup>th</sup>edn, J. Willey
- 11. R.T. Morrison and R.N. Boyd, Organic chemistry, 6<sup>th</sup>edn, Prentice hall of India, New
- 12. B. Dinda, Essential of Pericyclic and organic photochemistry, Springer (2016).
- 13. J. Sing & J Singh, Photochemistry and pericyclic reactions, New Age International (Pvt. Ltd). 3<sup>rd</sup> Edition (2010).

# PHYSICAL CHEMISTRY - II PAPER – CHEM 803C

**Total Marks: 100 (Theory 70 + Internal Assessment 30)** 

# **Unit-I: Chemical Thermodynamics**

12 L

Nernst heat theorem and the third law of thermodynamics, Calculation of entropy changes in chemical reactions, Mathematical and thermodynamic probability. Entropy and probability. The free energy of a mixture. Dependence of thermodynamic functions on composition. Partial molar quantities.

Thermodynamic properties of gases with special reference to real gases in the pure state and in mixtures. Concept of fugacity.

Analytical form of the chemical potential in ideal solutions. Chemical potential of the solute in a binary solution Application of Gibbs-Duhem equation.

The concept of activity:the rational concept and the practical concept. Colligative properties and activity of solute. Activities and reaction equilibria, experimental determination of activity coefficients of non-electrolytes, Numerical problems.

# **Unit -II: Adsorption and Aggregation:**

12 L

Surface tension and surface free energy; Pressure across an interface: Laplace equation, Kelvin equation; Wetting: Young-Dupre equation; Adsorption in liquid systems: Gibbs adsorption isotherm; Adsorption on solids: Langmuir isotherm, BET isotherm.

Surfactants, classification of surfactants, hydrophobic interaction, aggregation/micellization of surfactants, critical micelle concentration (cmc), factors affecting the cmc, thermodynamics of Micellization: phase separation and mass action models. concentration (CMC) of surfactants, thermodynamics of micellization. General experimental techniques employed in surfactant studies like tensiometry, conductometry, viscometry, spectrophotometry.

Brief introduction to soaps and detergents, their performance in soft and hard water conditions

# **Unit -III: Spectroscopy –II**

12 L

**NMR Spectroscopy:** Theory for NMR Population of energy levels. Larmor precession. Relaxation times: spin - lattice relaxation, spin-spin relaxation. Fourier transform spectroscopy in NMR .Chemical shift.Shielding and de-slielding mechanism.Fine structure, spin-spin splitting, coupling constant.Strongly coupled systems, shift reagent in NMR.Hyperfine structure. Nuclear overhauser effect (NOE), 1H and <sup>13</sup>C NMR. Two-Dimentional NMR.Chemical analysis by NMR techniques.

**ESR Spectroscopy**: General background of ESR spectroscopy .Representation of ESR spectrum. 'g' - value, ESR spectra of simple organic free radicals; Hyperfine coupling, prediction of expected number of lines and their relative intensities, ESR spectra of transition metal complexes, metal- hyperfine coupling, anisotropic ESR spectra, zero field splitting, application of ESR spectroscopy examples.

# **Unit -IV: Spectroscopy –III**

12 L

**Photoelectron Spectroscopy (PES):** Frank- Condon principle, Basic principles of photoelectron and X-ray photoelectron spectroscopies and their applications for chemical analysis of surfaces; application of ESCA and Auger spectroscopy for the studies of solids.

**NQR**: Nuclear quadruple resonance, Energy levels of a nucleus in a non-uniform electric field. Quadruple coupling constant. NQR spectra of molecular compounds.

*Mossbauer Spectroscopy*: Principles of Mossbauer spectroscopy, Doppler shift, Application of Mossbauer spectra for chemical structure determination, Numerical problems.

# **Suggested reading:**

- 1. G.W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
- 2. P. W. Atkins & J. de Paula, Physical Chemistry (8th edn.), OUP (2006). Oxford University Press.
- 3. K. Zeemanski, Thermodynamics.
- 4. N.K.Adams, Physics and Chemistry of Surface,
- 5. A.W.Adamson, Physical Chemistry of Surface,
- 6. M.J.Rosen, Surfactants and Interfacial Phenomena, (1978) John Willey, New York.
- 7. Y.Moroi, Micelles: Theatrical and Application Aspects, (1992) Plenum Press, New York
- 8. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th edn., Tata McGraw-Hill, New Delhi (2002).
- 9. D. A. McQuarrie and J.D. Simon, *Physical Chemistry*, VIVA Students Ed. (2003)
- 10. J. D. Graybeat. *Molecular Spectroscopy*, McGraw-Hill International Edition

#### LABORATORY COURSE - II

PAPER: CHEM 804C (Organic Chemistry)

**Total Marks: 150 (Theory 105 + Internal Assessment 45)** 

Credit: 06

- 1. Separation, purification and identification of compounds of binary solid mixtures by systematic qualitative analysis using different separation techniques like chromatographic techniques, steam distillation, fractional crystallization and sublimation
- 2. Identification of organic liquid compounds by distillation followed by systematic qualitative analysis
- 3. Organic preparation involving rearrangement reaction, condensation, nucleophilic substitution, heterocycles synthesis and multicomponent reactions.
- 4. Organic estimation Estimation of glucose, glycine, formic acid and acetic acid in vinegar.

# **Suggested Text and reference books:**

- 1. Practical Organic Chemistry, A. I. Vogel, ELBS, 2002.
- 2. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley Eastern, 1980.
- 3. Comprehensive Practical Organic Chemistry: Qualitative Analysis, V. K. Ahluwalia and S. Dhingra, Universities Press (India) Ltd, 2000.
- 4. N. K. Visnoi, Advanced organic Chemistry practical
- 5. R. K. Bansal. Laboratory Manual of Organic Chemistry (3rd edn.), Wiley-Eastern (1994).
- 6. R. G. Brewster & W.E. Mcwedn. *Unitized Experimental Organic Chemistry* (4th edn.), East-West Press (1977).

# **Electives**

PAPER: CHEM 805E (Bio-inorganic Chemistry)
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

Unit I: 5L

**Calcium in Biology**: Biochemical role of calcium, Storage and transport of calcium, Role of Ca<sup>2+</sup> in muscle contraction, Blood clotting mechanism, Biological calcification.

Unit II: 5L

Metallo-proteins and Metallo-enzymes of Fe: Ferritin, Transferrin, bio-mineralization and Siderophores, Peroxidase, Catalase, Hemerythrin, Cytochromes, Cytochrome P-450, Iron sulphur proteins, Rubredoxins, Ferredoxins.

Unit III: 5L

**Metallo-enzymes and proteins of copper and zinc**: Blue-copper proteins, Ceruloplasmin, Hemocyanin, Cytochrome-c oxidase, Superoxide dismutase, Carbonic anhydrase, Alcohol dehydrogenase, Carboxy peptidase, Metallothionein, inter changeability of Zn and Co in enzymes.

Unit IV:

**Biochemical role of Co, Mo and Mn**: Biological nitrogen fixation, Vitamin  $B_{12}$ ,  $B_{12}$ coenzyme, Cobalamines, Xanthine oxidase, Sulphite oxidase, Nitrite reductase, Arginase, Mn-SOD, Chlorophyll, Photosystem I and II, cleavage of water.

**Metals in medicines:** Toxicity of Hg, Cd, Pb, Cr, Be, Se, and As. Biological defence mechanism, Chelation therapy, Metals in diagnosis and Chemotherapy, Pt- complexes as anticancer drugs, Metal complexes as drugs.

#### **Suggested Reading:**

- 1. Bioinorganic Chemistry, Asim K. Das. Books & Allied Ltd, 2013
- 2. Bioinorganic Chemistry (Bertini, Ivano G, Harry B, Lippard, S. J, Valentine, J.S.), University Science Books, CA, 1994.
- 3. J.A. Cowan, Inorganic Biochemistry: An Introduction, 2<sup>nd</sup> Edition, Wiley-VCH, 1997
- 4. R. P. Hanzlik, Inorganic Aspects of Biological and Organic Chemistry,, Academic Press, New York, 1976

# PAPER – CHEM 806E (Bio-organic Chemistry) Total Marks: 50 (Theory 35 + Internal Assessment 15) Credits: 02

Unit I:

Chemistry of amino acids and peptides: Introduction to amino acids, nomenclature of  $\alpha$ -amino acids; structures, properties and synthesis of natural peptides and peptide synthesis, different strategies in peptide synthesis, solid phase methods; sequencing of polypeptides; preliminary concept of protein and their structures; protein denaturation; biosynthesis of amino acids.

Unit II:

Structure and function of sugar derivatives -deoxy, amino, branched chain sugars; Disaccharides (sucrose, maltose, lactose); carbohydrate metabolism; role of sugars in biological recognition. Polysaccharides of biological importance, dextran, sialic acid and cyclodextrin

Unit III: 6L

Classification of lipids, biological importance of fatty acids and lipids, essential fatty acids:  $\omega$ -3and  $\omega$ -6 fatty acids; Oxidation of fatty acids (alpha, beta, and omega), ketone bodies, fatty acid metabolism; Structure, sources and functions of prostaglandins, biosynthesis of prostaglandins, inhibition of prostaglandin synthesis; Synthesis of prostaglandins (PGE<sub>2</sub>, PGE<sub>3</sub> PGF<sub>2</sub> and PGF<sub>3</sub>).

Unit –IV:

Structure, functions and stability of some macrocyclic compounds, synthesis and different strategies adopted in the synthesis of exaltone, civetone and muscone.

# **Suggested Readings:**

- 1. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, (2001) Oxford Univ. Press, Oxford.
- 2. G. C. Barrett and D. T. Elmore, Amino acids and peptides (2004), Cambridge University press.
- 3. F. D. Gustone, Fatty acid and Lipid Chemistry (1996), Wiley
- 4. S. P. Bhtani, Chemistry of Biomolecules (2010), CRC Press
- 5. Chemistry of Biomolecules: An Introduction, R. J. Simmonds, RSC, 1992.
- 6. Lehninger Principles of Biochemistry, David L. Nelson and Michael M. Cox. 7<sup>th</sup> Edition. W H Freeman & Co (Sd). 2017.
- 7. Biochemistry, C.B. Power and G.R. Chatwal. Himalayan Publishing House. 4<sup>th</sup> edition 1999.
- 8. J.E Vance, D.E Vance, Biochemistry of Lipids, Lipoproteins and Membranes. Amsterdam: Elsevier (2002).

# PAPER - CHEM 807E (Surface Chemistry) Total Marks: 50 (Theory 35 + Internal Assessment 15) Credits: 02

# **Unit –I: Adsorption isotherm:**

12 L

Thermodynamics of adsorption isotherm, Different adsorption isotherms, Adsorption at solid-liquid, liquid-gas, liquid-liquid interfaces, Effect of added electrolyte on the surface excess of ionic surfactants.

**Mixed surfactants:** Different types of mixed micelle, cmc of mixed micelle, Clint's equation for cmc, counter ion binding in mixed surfactants.

# **Unit –II: Solubilisation and emulsification:**

12 L

Solubilization and Emulsification by Surfactants: Factors determining extent of solubilization, formation of emulsions, factors determining emulsion stability, microemulsions, conductance behaviour of microemulsions and applications.

#### **Reference Books:**

- 1. N.K.Adams, Physics and Chemistry of Surface,
- 2. A.W.Adamson, Physical Chemistry of surface,
- 3. M.J.Rosen, Surfactants and Interfacial Phenomena, (1978) John Willey, New York.
- 4. Y.Moroi, Micelles: Theatrical and Application Aspects, (1992) Plenum Press, New York

# PAPER – CHEM 808E Quantum Chemistry Total Marks: 50 (Theory 35 + Internal Assessment 15) Credits: 02

# Unit -I: Quantum Chemistry-I

12 L

Interpretation of wave function (probability density). Box normalization. Superposition principle and expansion theorem. Derivation of the expression of  $L_z$  in polar coordinate system.  $P_x$ ,  $L_z$  and  $\hat{H}$  operators are Hermitian: Proof. Unitary and projection operators. Some important theorems. Schmidt orthogonalization. Dynamical variables and operators, dynamical states. Expectation value and average value. Linear vector spaces in quantum mechanics. Completeness theorem. Equations of motion of classical mechanics (in brief). Poisson bracket and Dirac's version of Correspondence principle. Ehrenfest theorem. Constants of motion.

The Heisenberg Uncertainty relations (<u>position and momentum</u>, angle and angular momentum, time and energy relations): <u>proof</u>. Commutability and compatibility. Complete set of commuting operators. Fourier transform. Wave packet. Momentum space wave function.

Angular momentum operators (single particle system). Step up and step down operators. Spin angular momentum operators. Angular momentum operators (many electron system) and their commutation with spin free Hamiltonian operator. coupling of angular momenta, L-S coupling and j-j coupling. Term symbols and spectroscopic states. Pauli spin matrices and anti-commutation relations.

#### **Unit -II: Ouantum Chemistry-II**

12 L

Time independent non-degenerate perturbation theory (RSPT). Application: ground state of He atom. Degenerate RSPT. Applications: Stark effect, normal and anomalous Zeeman effect. Rayleigh- Ritz variation principle.Linear variation method. Applications: ground state energy of Heatom, harmonic oscillator.

Time dependent RSPT (First order).Fermi-Golden rule. Born-Oppenheimer approximation(in detail). Antisymmetrized wave Function. Slater determinant and Pauli exclusion principle.

#### **Reference Books:**

- 1. L.I. Schiff, *Quantum Mechanics*, Third Edition, McGRAW-HILL BOOK COMPANY, 1985.
- 2. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3<sup>rd</sup> Ed.(1997) Oxford UniversityPress.
- 3. B.H. Bransden& C.J. Joachain, *Physics of Atoms and Molecules*, Longmann Scientific and Technical, 1994.
- 4. B.H. Bransden& C.J. Joachain, *Quantum Mechanics*, Second edition, low price edition, PEARSON Education, First Indian Reprint, 2004.
- 5. J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesely Publishing Company.
- 6. Eugene Merzbacher, Quantum Mechanics, Wiley International Edition, 1970.

#### SEMESTER III

# INORGANIC CHEMISTRY - III PAPER - CHEM 901C

Total Marks: 100 (Theory 70 + Internal Assessment 30) Credits: 04

# **Unit: I Reaction Mechanism of Transition Metal Complexes**

12L

Stepwise and overall formation constants, Factors affecting the stability of metal complexes, chelate effect, determination of binary formation constants, Energy profile of reactions, Labile and inert complexes; dissociative, associative and interchange mechanisms of ligand substitution reactions, mechanisms of ligand-replacement reactions, ligand substitution reactions in square planar and octahedral complexes, mechanisms of ligand-replacement reactions trans effect, acid & base hydrolysis; ; isomerisation and racemisation of tris-chelate complexes, Ray-Dutta and Bailar twist mechanisms. Mechanism of electron transfer (redox) reactions: inner and outer sphere reactions, complementary and non-complementary reactions, stereochemical non-rigidity and fluxional molecules

#### Unit II $\pi$ -Acid complexes and Clusters

12L

**Transition metal \pi-acid complexes:**  $\pi$ -acid ligands (CO, NO, tertiary phosphine, arsine), structure, bonding, synthesis and reactivity of complexes of CO, NO, tertiary phosphine, metal carbonyl hydrides.

# Metal carbonyls, clusters and Metal-metal multiple bond:

**Metal clusters**: Low nuclearity and high nuclearity carbonyl clusters; Boron clusters: Structure and bonding of boranes and Lipscomb's topology, styx system of numbering, nomenclature; Synthesis and structure of carboranes, metalloboranes, metallocarboranes; Skeletal electron counting, Wade's rule. Metal-metal multiple bond, quadruple bond, structures and bonding (MO).

# **Unit III: X-ray crystallography**

12L

*Crystals Lattices and symmetry:* Lattice points, Unit Cells, ; Symmetry operations and elements of symmetry, Point groups, Classification of unit cells, Crystal systems, Herman-Mauguin notation, Bravais Lattices, Distinction between trigonal and hexagonal systems, Crystal planes and indices Law of rational indices.

*Space groups and equivalent positions:* Screw axis, Glide planes, Space groups, Relationship between space groups, point groups, Equivalent positions, Special positions,

**X-ray diffraction:** and Bragg's law; Crystal systems and symmetry, point groups, stereographic projection of 32 point groups and space groups-Hermann–Mauguin notations,; Primitive and non-primitive unit cells; Symmetry elements: isogonal symmetry groups and reciprocal lattice.; X-ray-instrumentation Data collection, data reduction, refinement and structure solution

# **Unit IV Transition metal chemistry:**

12L

**Inner transition Metals:** comparative study of Lanthanides and Actinides with reference to oxidation states, complex formation, magnetic properties, colour and spectral properties, Lanthanide shift reagents.

#### **Platinum Metals:**

General discussions: position in periodic Table, electronic configurations, oxidation states, general trends in properties, Important compounds of Ruthenium, Rhodium, Iridium, osmium, palladium and platinum- synthesis, structure, properties and applications...

# **Suggested Readings:**

- 1. Advanced Inorganic Chemistry. F.A.Cotton, G. Wilkinson, C.A.Murillo and M. Bochmann, 5<sup>th</sup> Edition, Wiley Interscience, N.Y
- 2. J. Huhee, E.A. Keiter, R.L. Keiter& O.K. Medhi-Inorganic Chemistry-Principles of Structure and Reactivity, 5<sup>th</sup>Edn..Pearson Education, 2007.
- 3. Crystal Structure Determination, William Clegg, Oxford University Press, 1998.
- 4. Structure Determination by X-ray Crystallography, Mark Ladd and Rex Palmer (September 30, 2003).
- 5. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
- 6. Shriver & Atkins Inorganic Chemistry, Atkins, Overton, Rourke, Weller, Armstrong, South Asia Edn. 5th Edn. Oxford University Press, 2010.
- 7. N. N. Greenwood & A. Earnshaw. Chemistry of the Elements, Pergamon Press (1984).
- 8. F. Basolo & R. G. Pearson, Mechanism of Inorganic Reactions, Wiley Eastern (1967)

# ORGANIC CHEMISTRY – III PAPER - CHEM 902C

Total Marks: 100 (Theory 70 + Internal Assessment 30) Credits: 04

# Unit I: Nuclear magnetic resonance spectroscopy for organic compounds 16L

Relaxation phenomenon in NMR, broadening of signals, sample handling and solvent for NMR study, chemical shift, internal standards, factors affecting the chemical shift, spin-spin coupling, multiplicity of splitting and relative intensity of lines, coupling constant, first order and non-first order splitting, vicinal and geminal coupling, long range coupling – two bond coupling (2J) three bond coupling (3J), Nuclear overhauser effect (NOE), Karplus relationship. Designation of spin systems. Chemically induced dynamic nuclear polarization (CIDNP). Interpretation of PMR spectra. <sup>13</sup>C NMR spectroscopy: Principle, multiplicity, proton –decoupling, off-resonance decoupling, noise-decoupling, <sup>13</sup>C chemical shifts values, DEPT and INEPT terminology; Two dimensional NMR spectroscopy: magnetic resonance imaging (MRI). Applications of NMR in the structure elucidation of organic compounds.

# **Unit II: Mass spectroscopy for organic compounds**

8L

Introduction – basic theory, instrumentation and sample handling. Methods of generation of mass ions – electron impact (EI), chemical ionization (CI), electron spray ionization (ESI) and fast atom bombardment (FAB) techniques, TOF-MALDI and SELDI; Tandem mass spectroscopy, general mass fragmentation pattern of organic compounds, base peak, molecular ion, relative intensity, mass ions fragmentation, metastable ions, even electron rule, nitrogen rule, HDI, application of mass spectroscopy.

# **Unit III: Main group Organometallic Chemistry:**

12L

Introduction, importance of organometallic compounds as reagents, additive and catalyst. Chemistry of organolithium, magnesium, zinc, copper, aluminium, cadmium and mercury synthesis, structures and reactivity. Stability, preparation and reactivity of metal alkyls, aryls and hydrides. Applications of main group organometallics in organic synthesis.

# Unit IV: Transition metal based Organometallics in organic synthesis 12L

General- Ligands, bonding, haptonumber, stability, synthesis and reactivity. Uses of Organo-transition metal reagents of chromium, cobalt, iron, nickel, rhodium and palladium in organic synthesis; sandwich compounds and their reactivity, Tebbe reagent.

Synthesis and reactions of cyclopentadienyl metal carbonyls, cyclopentadienyl metal hydrides, cyclopentadienyl metal halides, arene metal group complexes,  $\eta$ 6-arene-chromium tricarbonyl in organic synthesis

**Palladium catalyzed C–C coupling reactions**: The Heek reaction, Suzuki-Miyaura coupling, Sonogashira coupling, Stille coupling, Kumada coupling, Negishi coupling.

# **Suggested readings:**

- 1. High-Resolution NMR Techniques in Organic Chemistry, Third Edition, 2016, by Timothy D.W. Claridge, Oxford, United Kingdom. Published by Elsevier Ltd.
- 2. Organic Spectroscopy- Principles and Applications, Jag Mohan, Narosa publishing House.
- 3. Spectroscopic Methods in Organic Chemistry, By D.H. Williams, I. Fleming. Tata McGraw Hill Pub. Co. Ltd.
- 4. Organic Spectroscopy, 3<sup>rd</sup> Edn, By William Kemp. Published by Palgrave, New York.

- 5. The Organometallic Chemistry of The Transition Metals. By Robert H. Crabtree, Yale University, New Haven, Connecticut. Published By John Wiley & Sons, Inc., Hoboken, New Jersey. Isbn 0-471-66256-9.
- 6. Organometallics in Synthesis A Manual. Edited by Manfred Schlosser. Published by John Wiley & Sons Ltd.
- 7. Handbook of Functionalized Organometallics Applications in Synthesis. Volume -1 By Paul Knochel. Published by Wiley-VCH Verlag GmbH & Co.
- 8. Metallo-Organic Chemistry. By A.J. Pearson. John Wiley & Sons.
- 9. Organotransition Metal Chemistry : Applications to organic synthesis, Stephen G Davies Pergman Press
- 10. Organolithiums: Selectivity for synthesis, Jonathan Clayden, Pergamon, 2002
- 11. R O C Norman and J M Coxon, Principles of organic synthesis, 3<sup>rd</sup> Edition, CRC Press.

# PHYSICAL CHEMISTRY - III PAPER – CHEM 903C

Total Marks: 100 (Theory 70 + Internal Assessment 30) Credit: 04

# **Unit -I: Polymer Chemistry**

12 L

Polymer and Characterisation:-Banz concepts of polymer science, Molecular forces and chemical bonding in polymers.Polymer solution and fractionation. Gel permeation Chromatography and molecular weight determination by viscometry, osmometry, light scattering and ultra centrifugation, molecular weight distribution curve.

Polymerization:- mechanism and kinetics of step growth and chain growth polymerization- radical, ionic and ring opening polymerization, copolymerization, polymerization techniques and polymer reaction, polymer structure and physical properties: configuration of polymer chain crystal structure of polymers: speciality polymers: Block copolymer, polymer colloids and biomedical polymers.

#### **Unit -II: Chemical Kinetics-II:**

12 L

Theory of reaction rates; Temperature effect on reaction rates; Rate constant for simple; Bi-molecular reactions; Collision theory; Activated complex theory.Reactions in solutions: Diffusion controlled and activation controlled reactions; Thermodynamic formulation of rate constant: effect of pressure & ionic strength; Reaction in surfaces: Langmuir adsorption isotherm; kinetics of surface catalyzed uni-molecular and bimolecular reactions; Applications in ammonia synthesis and oxidation of carbon-monoxide.

#### **Unit -III: Electrochemistry-I:**

12 L

Activity in electrolytic solutions. Freezing point depression and the mean ionic activity coefficient. The Debye-Huckel theory for dilute ionic solutions (derivation) and correction for concentrated solutions Equilibrium in ionic solutions. Ion association.

# **Unit -IV: Solid State Chemistry:**

12 L

Review of the basic concepts: Bragg's law, Miller indices, Elements of symmetry (plane, axis and centre of symmetry). X-ray diffraction: powder method, principle and applications.

Crystal Defects: Point defects, Stoichiometric and non-stoichiometric defects, Kroger-Vink notation for crystal defects, thermodynamics of Schottky and Frenkel defect formation. Metals, insulators and semiconductors; intrinsic and extrinsic semiconductors, p-n junction.

Solid Solutions: Substitutional, interstitial and subtractional solid solutions & distortions

#### Reference Books:

- 1. C. Tanford, Physical Chemistry of Macromolecules, Wiley, Newyork, 1961
- 2. V.R. Gowariker, Polymer Science, New Age International New Delhi, 1986
- 3. Y. Morai, Micelles: Theoretical and Applied Aspects, Plenum (1992).
- 4. G. Odien, Principles of Polymerization, 3 edition (1991) John Wiley & Sons, Singapore.
- 5. P. Bahadur and N.V. Sastry, Principles of Polymer Science, (2002) Narosa, New Delhi.
- 6. F.W. Billmayer, Jr., Text Book of Polymer Science, 3 Edition (1984), Wiley-Interscience, New York.
- 7. K.J.Laidler, Chemical Kinetics, 3<sup>rd</sup> Ed.(1967), Harper and Row Publishers, New York.
- 8. H. Eyring, S. H. Lin and S. M. Lin, *Chemical Kinetics* (1999), Jhon Willey, New York.
- 9. J.O'M, Bockris and A.K.N. Reddy, *Modern Electrochemistry*, Vol.1&2 (1998), Plenum Press, New York.
- 10. A. R. West Solid State Chemistry and its Applications, John Wiley (2001).
- 11. Crystal Structure Analysis, Jenny Glusker and Kenneth Trueblood (August 1992).
- 12. N. B. Hannay. Solid State Chemistry, Prentice-Hall (1979).
- 13. D. K. Chakraborty. Solid State, New Age International, New Deldi (1996)

#### LABORATORY COURSE-III

Paper: CHEM 904C (Physical Chemistry)

Total Marks: 150 (Practical 105 + Internal Assessment 45)

Credit: 06

# **Laboratory Course in Physical Chemistry**

- 1. Determination of specific rotation of cane sugar and determination of concentration of supplied sample.(Quantitative-one day).
- 2. Potentiometric titration of Co(II) by  $K_3[Fe(CN)_6]$  and determination of concentration of Co(II) in a solution. (Quantitative-one day).
- 3. Conductomectric titration of triple mixture containing KCl, NH<sub>4</sub>Cl and HCl by AgNO<sub>3</sub> and by NaOH solution. (Quantitative-one day).
- 4. Verification of Beer's law and determination of concentration of unknown solution spectrophotmetrically(Quantitative-one day).
- 5. Determination of strengths of halides in a mixure ,potentiometrically.
- 6. Determination of pH of buffer solutions and hence to calculate the E<sup>0</sup> of quinhydrone electrode
- 7. Spectrophotometric determination of pKa of an indicator in micellar and microemulsion media.
- **8.** Determination of specific rotation of sucrose and rate constant of its hydrolysis using a polarimeter.
- 9. Determination of rate constant and order of the reaction between KBrO<sub>3</sub> and KI in acid medium.(Qualitative- one day)
- 10. Kinetic study of decomposition of K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> by KI and effect of added salt. (Qualitative- two day)
- 11. Determination of formula of cupro-ammonium ion. (Qualitative- one day)
- 12. Determination of standard electrode potential of quinhydrone electrode. (Qualitative-one day).

- 13. Determination of composition and stability constant of Ferric-salicylic acid complex by Job's method. (Qualitative-two day).
- 14. Determination of critical micellarconcentration(CMC) of sodium lauryl sulphate from the measurement of conductivities at different concentrations.

#### **Reference Books:**

- 1. D. P. Shoemaker, C. W. Garland & J. W. Nibler. *Experiments in Physical Chemistry* (5<sup>th</sup>edn.), McGraw Hill (1989)
- 2. Findlay's Practical Physical Chemistry, 9<sup>th</sup> Ed. Revised by B.P. Levitt, Longman.1973.
- 3. V. D. Athawala& P. Mathur. *Experimental Physical Chemistry*, New Age International Publishers (2001).

#### **ELECTIVES**

# PAPER - CHEM 905 E

Special Topics in Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

# **Unit-I: SUPRAMOLECULAR CHEMISTRY**

12L

Concepts and Languages of supramolecular chemistry - Molecules, super molecules; factors leading to strong binding (non-covalent interactions); molecular receptors – design and principles; Types of supramolecular interactions (Hydrogen bonding, vander Waal's interaction,  $\pi$ -stacking, CH- $\pi$ , anion- $\pi$  interaction). Supramolecular chemistry in inorganic perspective: Inorganic crystal engineering and design principle of metal organic framework (MOF) and inorganic-organic hybrid material. Types of interactions between host and guest molecules; Thermodynamics of hostguest complexation; Enthalpy and entropy contributions, complexation free energies; Molecular recognition - factors involved; Molecular receptors - for alkali metal ions, ammonium ions, anions and neutral molecules. Crownethers, cryptands, spherands and ionophores; Creation of rotaxanes, catenanes and cyclophanes; Supramolecular catalysis- Catalysis by Reactive Macrocyclic Cation Receptor Application supramolecular chemistry catalysis, delivery, of in drug recognition/sensing and material science.

#### **Unit –II: NANO CHEMISTRY**

12L

Background to Nano-science and Technology - Implications for Physics, Chemistry, Biology and Engineering - Classifications of nanostructured materials - nano particles - quantum dots, Nanowires, nano-tubes – ultra – thinfilms – multilayered materials; Typical syntheses of nano particles, oxide nano tubes and fibres, metal nano particles; Length Scales involved and effect on properties: Mechanical, Electronic, Optical, Magnetic and Thermal properties.

Synthesis of nanoparticle: Bottom-up Synthesis -Top-down Approach: Precipitation, Mechanical Milling, Colloidal routes, Self-assembly, Vapour phase deposition, MOCVD, Sputtering, Evaporation, Molecular Beam Epitaxy, Atomic Layer Epitaxy, MOMBE.

Characterization of nano particles- X-ray diffraction technique, Scanning Electron Microscopy - environmental techniques, Transmission Electron Microscopy including high-resolution imaging, Surface Analysis techniques

Application of nano-structured material in organic synthesis, dendrimers, bucky balls and nano tubes (properties and applications), drug delivery systems; Nanotechnology for sustainability, Nanomedicine, Environmental, health, and safety issues Suggested reading:

- 1. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
- 2. A.S. Edelstein and R.C. Cammearata, eds., Nanomaterials: Synthesis, Properties and Applications, (Institute of Physics Publishing, Bristol and Philadelphia, 1996)
- 3. N John Dinardo, Nanoscale charecterisation of surfaces & Interfaces, Second edition, Weinheim Cambridge, Wiley-VCH, 2000
- 4. G Timp (Editor), Nanotechnology, AIP press/Springer, 1999
- 5. AkhleshLakhtakia (Editor) The Hand Book of Nano Technology, "Nanometer Structure", Theory, Modeling and Simulations. Prentice-Hall of India (P) Ltd, New Delhi, 2007.
- 6. Desiraju, G. R. Crystal Design: Structure and Function, (John Wiley & Sons, 2003).
- 7. Steed, J. W.; Atwood, J. L. Supramolecular Chemistry, (John Wiley & Sons, 2009).

# PAPER: CHEM 906E Chemistry of Natural products

**Total Marks: 50 (Theory 35 + Internal Assessment 15)** 

Credits: 02

UNIT - I

**General:** Sources and types of natural products, method of isolation and structure elucidation, importance of natural products, biosynthesis of some common type of natural products *viz.* terpeneoids, steroids, flavonoids and alkaloids.

UNIT- II 6L

**Chemistry of terpenoids**: General methods of determining structure, correlations of configurations, sesquiterpenoids, diterpenoids, triterpenoids with special reference to the isolation, structure and stereochemistry. Chemistry of Caryophyllene and isocaryophyllene, abietic acid and Gibberellic acid.

UNIT- II 6L

**Alkaloids and Phenolics** - Chemistry of quinoline, isoquinoline, phenanthrene and indole group of alkaloids - papaverine, cimchonine quinine, morphine, thebaine, codeine, reserpine with special reference to isolation, structure and stereochemistry. Plant phenolics with special reference to the general structures, reactions and synthesis of anthocyanins, anthocyanidins, flavones flavonols, isoflavones, chalcones, coumarins, quinines and tannins.

UNIT IV 6L

*Steroids and hormones:* Classification and nomenclature of steroids, Structure, spectral properties of steroids, stereochemistry of steroids, reaction of steroids, chemistry of cholesterol, ergosterol, vitamin D, bile acids, steroid hormones- oestrone, progesterone, testosterone., artificial hormones, Miscellaneous transformations of steroid molecules- steroidal glycosides and alkaloids.

#### **Reference books:**

- 1. Organic Chemistry, I.L. Finar, volume 2, ELBS, 5<sup>th</sup> edition (1975).
- 2. Organic Chemistry. Morrison Boyd and Bhattacharjee, 7<sup>th</sup> edition (2013), Pearson.
- 3. Chemistry of Plant Natural Products Stereochemistry, Conformation, Synthesis, Biology, and medicine. Vol 1 and Vol 2. Springer Heidelberg New York Dordrecht London. 2015

#### PAPER: CHEM 907E

# **Environmental and Green Chemistry**

Total Marks: 50 (Theory 35 + Internal Assessment 15) Credits: 02

# **Unit – I: Environmental Chemistry**

12L

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, Ozone depletion, The green-house effect and Global warming, El-Nino phenomenon. Micro-organism in aquatic chemical reactions, Eutrophication, Re-cycle of wastewater in process industry, Treatment of sewage and reuse of water in industry and agriculture, microbiologically mediated redox reactions and Nitrogen transformation by bacteria. Water pollutants: Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity, DO, BOD, COD etc.); industrial and waste-water treatment; Chemical hazards, chemical disaters, pollution of environment-man made, industrial, natural disasters, environmental biochemistry, toxicological chemistry; analysis of water and waste water, solid wastes and air pollution-Photochemical smog, Auto exhausts, Acid-rains, Air-quality standards. Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides, ozone, PAN, cyanide, pesticides, insecticides and carcinogens.

# **Unit – II: Green Chemistry**

12L

Definition, Concepts and basic principles of green chemistry, need of green chemistry, green chemistry as an alternative tool for reducing pollution, atom economy, less hazardous chemical syntheses, atom economy in rearrangements, addition and pericyclic reactions, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, Green synthesis, clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology. Development of new methods for organic synthesis such as Green Synthesis: use of sonochemistry, use of ionic liquids, use of microwaves, bio-catalysis. Selection of solvent: i) Aqueous phase reactions ii) Reactions in ionic liquids iii) Solid supported synthesis iv) Solvent free reactions, Green catalysts: i) Phase transfer catalysts (PTC) and ii) Biocatalysts. Microwave and Ultrasound assisted green synthesis: Aldol condensation, Cannizzaro reaction, Diels-Alder reactions, Strecker synthesis, Willaimson synthesis and Dieckmann condensation.

#### **Book Suggested:**

- 1. Handbook of Environmental chemistry, Springer-Verlag, O. Hutzinger.
- 2. M. Bernhard, F.E. Brinckman & P.J. Sadler. The Importance of Chemical Speciation in Environmental Processes, Springer-Verlag,
- 3. L.J. Fristschen, & L.W. Gay, Environmental Instrumentation, Springer-Verlag,.
- 4. Real World Cases in Green Chemistry, ACS, M.C. Cann & M.E. Connelly.
- 5. P.T. Enastas and T.C. Williamson, Green Chemistry: Designing Chemistry for Environment, ACS
- 6. Green separation processes, methods and application, Fonso, National Scientific Book Agency, Delhi-110053.

- 7. G.W. Vanloon, S.J. Duffer, Environmental Chemistry A Global Perspective, (2000) Oxford University Press.
- 8. F.W. Fifield and W.P.J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.
- 9. Colin Baird, Environmental Chemistry, (1995) W.H. Freeman and Company, New York.
- 10. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd., New Delhi.
- 11. Peter O. Warner, Analysis of Air Pollutants, 1st Edition (1996), John Wiley, New York.
- 12. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Estern Ltd., New Delhi.
- 13. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi

# PAPER - CHEM 908 E Advanced Group Theory Total Marks: 50 (Theory 35 + Internal Assessment 15) Credits: 02

# **Unit -I: Group Theory – I:**

12 L

The concept of groups; group multiplication tables and the rearrangement theorem; subgroups, classes and the related theorems; commutative groups (Abelian), cyclic group; isomorphism and homomorphism. Examples.

Molecular point groups (in Brief), similarity transformation and the invariance of characters of matrices under such transformation, matrix representation of point groups; reducible, irreducible and equivalent and inequivalent representations; the great orthogonality theorem (no derivation) and its corollaries, character tables, construction of character tables in complex cases such as  $D_{6h}$ ,  $T_detc$ ; the group of Schrodinger equation; basis function for irreducible representation "projection" operator; direct product representation .

# Unit -II: Group Theory - II (Physical Applications):

12 L

Symmetry factoring of secular equations; LCAO -MO ,II bonding and Huckel's theory ;some examples: ethylene ,bengene ,Naphthalein. symmetry based "selection rules" for cyclization reaction (Woodward Hoffmannrule) Hybrid orbital and Molecular orbitals for  $AB_n$  -type molecules. Crystal field theory (CFT) Splitting of energy levels, and terms in a chemical environment. Determining the symmetry types of the normal modes; selection rule for fundamental (infra-red and Raman) vibrational transitions. Mutual Exclusion rule.

# **Reference Books:**

- 1. Chemical Application of Group Theory F.A. Cotton,3<sup>rd</sup> edition, A Wiley Interscience publication
- 2. Group Theory and Quantum Mechanics, M.Tinkham, Tata McGraw Hill, publishing Ltd.
- 3. Group Theory and Chemistry, David M. Bishop, Clarendon Press Oxford.
- 4. Group Theory and its application to Physical Problem, M. Hamermeah, Dover publication.

#### **SEMESTER IV**

# INORGANIC CHEMISTRY-IV PAPER: CHEM 1001C

**Total Marks: 100 (Theory 70 + Internal Assessment 30)** 

Credits: 04

# **UNIT I - Basic Organometallic Chemistry:**

12L

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, Ligands in organometallic chemistry; Synthesis, bonding and reactivity of Metalalkyl, -alkene, -alkyne, -allyl, -carbene, -carbyne and -carbide complexes, Agostic interaction, Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples; Chemistry of  $\eta 3$  - $\eta 6$  cyclic,sandwich and half-sandwich transition metal complexes. Synthesis and reactions of cyclopentadienyl metal carbonyls, cyclopentadienyl metal hydrides, cyclopentadienyl metal halides, arene -metal complexes.

# **UNIT II - Catalysis Using Organometallic Compounds:**

16L

Terminology in catalysis (Turnover, Turnover number, Turnover frequency or turnover rate, mole fraction, eantioselectivity, stereoselectivity, chemoselectivity, regioselectivity); Catalytic Hydrogenation of alkenes and related reactions: Hydrogenation catalysts, Catalytic cycle of Wilkinson's catalyst, Catalytic asymmetric synthesis, the mechanism of asymmetric hydrogenation using a chiral catalyst.

**Olefin Metathesis**: synthesis of Grubbs' and Schrock catalysts, Mechanism of olefin metathesis, ring opening metathesis, cross metathesis, ring closing metathesis, ring opening polymerization metathesis, acyclic diene metathesis polymerization, enyne metathesis

Olefin polymerization and oligomerisation reactions: The Ziegler-Natta catalyst, site control and chain end control mechanisms, metallocene based catalysts, post metallocenes catalyst.

# **UNIT III Inorganic polymers:**

8L

Classification of inorganic polymer, inorganic polymerisation reactions (addition, condensation and coordination polymerisation). Polysiloxanes, polysilanes, poly phosphazenes, polymeric sulfur;

**Coordination Polymers:** Definition, classification and design strategies, network topologies, supramolecular isomerism, interpenetration, porous coordination polymers, properties and applications

# **Unit IVInorganic Photochemistry**

12L

Introduction to inorganic photochemistry, photophysical and photochemical characteristics of the electronically excited states of inorganic compounds, ligand field states, Selection charge transfer states; Photochemical processes: rules. Jablonski diagram, Fluorescence and phosphorescence, delayed fluorescence, Photochromism, Photosensitization, Quantum yield; Photochemical reactions: substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes; Application of inorganic photochemistry: Molecular recognition, Sensing, Photochemical splitting of water, Dye sensitized solar cells.

# **Suggested Reading:**

1. Organometallic Chemistry- A Unified Approach, R. C. Mehrotra. And A.Singh, New Age International, Ltd. New, Delhi.

- 2. Advanced Inorganic Chemistry. F.A.Cotton, G. Wilkinson, C.A.Murillo and M. Bochmann, 5<sup>th</sup> Edition, Wiley Interscience, NewYork.
- 3. N. N. Greenwood & A. Earnshaw. Chemistry of the Elements, Pergamon Press (1984.
- 4. Shriver & Atkins Inorganic Chemistry, Atkins, Overton, Rourke, Weller, Armstrong, South Asia Edn. 5th Edn. Oxford University Press, 2010.
- 5. Fundamentals of Photo chemistry, K.K.Rohatgi- Mukherjee, New Age International Publishers, New Delhi
- 6. A.W. Adamson & P.D. Fleischauer. Concepts of Inorganic Photochemistry, John Wiley & Sons (1975).

# ORGANIC CHEMISTRY – IV PAPER: CHEM 1002C

Total Marks: 100 (Theory 70 + Internal Assessment 30) Credits: 04

# **Unit I: Heterocyclic chemistry**

12L

Hantzsch-Widman nomenclature for monocyclic, fused and bridged heterocycles; Basicity and aromaticity of heterocycles; Synthesis, properties and reactions (ring openings & heteroatom extrusion) of 3- membered heterocycles (aziridines, oxiranes and thiiranes), 4- membered heterocycles (azetidine, oxetanes and thietanes); Synthesis and reactivity of azoles (imidazole, pyrazole, oxazole, isoxazole, thiazole, isothiazole and their benzo derivatives) and azines (6-membered heterocycles with two hetero atoms -pyridazines, pyrimidines and pyrazines), caffeine; theobromine and theophylline.

#### **Unit II: Nucleic acids and enzymes**

12L

Introduction, nucleic acid bases, Purine and pyrimidine bases of nucleic acids, nucleosides and nucleotides, their structures and nomenclature, structures and functions of NADH, NADP and ATP, Structures of RNA and DNA; DNA base-pairing, double helical structure of DNA, replication of DNA and mutagenesis, codon, anticodon, t-RNA, structure and genetic code, transcription and translation

Enzymes: nomenclature, stereochemical aspects, Mechanism of enzyme action, kinds of reactions catalyzed by enzymes, cofactors, co-enzyme chemistry. **Application and enzyme catalytic organic reactions** – Oxidation, reduction, isomerization, epimerization, hydrolysis, phosphorylation, acylation, methylation, decarboxylation, dehydration. Enzymatic hydrolysis of peptides (carboxy peptidase, trypsin, chrymotrypsin and Lys C);

# Unit III- Drugs and drug design:

14L

Concepts of drugs, classification, analogues and pro-drugs, theories of drug action, assay and metabolism of drugs; Drug design, theory of drug design, structure activity relationship (SAR), Quantitative structure activity relationship (QSAR); prodrugs and soft drugs; ADME.

# Synthesis and uses of the following drugs of different pharmacological activities:

- a) Antimalerials: Quinine, chloquine, Trimethoprim
- b) Analgesic & Antipyretics: Paracetamol, Meperidine, methadone, Aminopyrine.
- c) Anti-inflammatory: Aspirin, Ibuprofen, Diclophenac, Indomethacin, coxib
- d) Antitubercular and antileprotic: Ethambutol, Isoniazide&Dapsone

- e) Anaesthetics: Lidocaine, Thiopental.
- f) Antihistamines: Phenobarbital, Diphenylhydramine.
- g) Tranquilizers: Diazepam, Trimeprazine
- h) Cardiovascular: Synthesis of dilliazem, quinidine, methyldopa, atenolol, oxyprenol

# **Unit IV: Chromatography and optical microscopy:**

10L

Basic concept of chromatographic separation – adsorption and partition chromatography, theory and handling of different chromatographic techniques – thin-layer, column, and paper chromatography; Gas chromatography: Basic principle, basic instrumentation, column types and column selection; detectors (FID, TCD, ECD, NPD); sample separation and applications. High performance liquid chromatography (HPLC): Instrumentation - basic equipment; pumping and injection system, column and its packing materials, normal and reverse phases; detectors, sample separation and application. Gel permeable (filtration) chromatography, Size exclusion chromatography, Gel electrophoresis.

**Optical microscopy**: Optical Rotatory Dispersion and Circular Dichroism: Definition, Deduction of absolute configuration, octane rule for ketones.

#### **Recommended text and reference books:**

- 1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V.Gupta, Springer Verlag.
- 2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
- 3. Heterocyclic chemistry J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
- 4. Heterocyclic Chemistry, T.L. Gilchrist, Pearson Education
- 5. Lehninger Principles of Biochemistry, David L. Nelson and Michael M. Cox. 7<sup>th</sup> Edition. W H Freeman & Co (Sd). 2017.
- 6. Bioorganic and Bioinorganic and Supramilecular Chemistry. P.S. Kalsi, New Age International (Pvt. Ltd.) 2<sup>nd</sup> edition 2010.
- 7. A. Kar, Medicinal Chemistry, New Age publication
- 8. Thomas Nogrady, Donald F. Weave, Medicinal Chemistry-A Molecular and Biochemical Approach, Oxford University Press.
- 9. Burger. Medicinal Chemistry and Drug Discovery, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
- 10. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-Hill (2005).
- 11. S. S. Pandeya& J. R. Dimmock.Introduction to Drug Design, New Age International.(2000).
- 12. D. Lednicer. Strategies for Organic Drug Synthesis and Design, John Wiley (1998).
- 13. Graham & Patrick. Introduction to Medicinal Chemistry (3rd edn.), OUP (2005).
- 14. Principles and Practice of Modern Chromatographic Methods, (1st Edition), Robards, Jackson & Haddad, Academic press (1994).
- 15. Chromatographic Methods (5<sup>th</sup> Edn), A. Braithwaite, J.F. Smith, Kluwar Academic Publisher.

# PHYSICAL CHEMISTRY - IV PAPER – CHEM 1003C

Total Marks: 100 (Theory 70 + Internal Assessment 30) Credit: 04

#### **Unit - I. Statistical Thermodynamics**

12 L

Independent subsystems and distinguishability.Boltzmann distribution (nondegenerate and degenerate cases). Review of partition function: Thermal De Broglie wavelength. Partition functions for electronic, nuclear, rotational and vibrational degrees of freedom. Thermodynamic quantities in terms of partition functions.Entropy of ideal gas.Gibbs paradox. Equilibrium constants (ideal gas reaction) in terms of partition function.

The mathematical proof of the equipartition of energy principle. Specific heats of solids, fluctuations.

# **Unit - II : Photochemistry**

12 L

# Physical properties of excited molecules:

Nature of changes on electronic excitation, Potential energy diagram, Absorption band shape and Franck-Condon Principle, Emission Spectra, Environmental effects on absorption and emission properties, Excited state dipole moment, Redox potential and acidity constants of aromatic acids. Polarisedluminencence, non radiative intra-molecular electronic transition, internal conversion, intersystem crossing, crossing potential energy surface (Franck-Condon factor).

# Photo-physical processes in excited state:

Types of photophysical pathways, Radiationless transitions, Fluorescence emission, Triplet state and phosphorescence emission, Fluorescence quenching, Stern-Volmer equation, Concentration quenching and excimer formation, Quenching by foreign substrates, Exciplex formation. Mechanism of quenching, energy transfer process (Forster dipole coupling), electron transfer phenomenon (Marcus theorem, Rehm Weller theorem), eximer. Laser

# **Unit -III: Bio-physical Chemistry:**

12 L

Hydrophobic effect and self organising systems, structure and functions of proteins and nucleic acids and their stability. Structure and functions of cell membranes; Ion transport through cell membranes and nerve conduction; Multiple equilibria; stacking and cooperative interactions in biological systems. Muscle contraction; Techniques for study of structure and functions of proteins and nucleic acids.

# **Unit -IV: Electrochemistry–II:**

12 L

Electrodics - The basic electrodic equation: Butler-Volmer equation, overpotential, polarisable and non-polarizable interfaces; Faradaic and non-faradaic Currents, Over-potentials, aspects of deviation from equilibrium. Electrical conductance of solutions; The Debye HuckelOnsagarequation for conductance (derivation); Conductance at high fields and high frequencies, Conductance in non-aqueous solvents. Fuel Cells: H<sub>2</sub>-O<sub>2</sub> cell, Air-H cell; Electricity producing cells: Na-S, Sb-S.

# Numerical problems.

Reference books:

- 1. D. A.McQuarrie, Statistical Mechanics, (2003), Viva Books Pvt. Ltd. New Delhi.
- 2. M. C.Gupta, *The Statistical Thermodynamics*,(1990), New Age International (P) Ltd. New Delhi.
- 3. M.Dole, Introduction to Statistical Thermodynamics

- 4. K.K.Rohtagi-Mukherjee, *Fundamental of Photochemistry*,(1986) New Age International New Delhi.
- 5. J. G. Calvert and J. N. Pitts, Jr., *Photochemistry* (1966) John Wiley & Sons, New York.
- 6. R. P. Wayne, *Principles and Application of Photochemistry* (1988), Oxford University Press, Oxford.
- 7. N. J. Turro, Modern Molecular Photochemistry, (1991) Univ. Science Books, Sansalito.
- 8. J. F. L Lakowicz, *Principles of Fluorescence Spectroscopy*, 2<sup>nd</sup>Edn. (1999) Planum Publishers, New York.
- 9. L. Lehninger. *Biochemistry*, 8th edition, Kalyani Publishers (2008).
- 10. G. Thomas. Medicinal Chemistry: An Introduction, 2nd Edition, Wiley (2007).
- 11. S. P. Bhtani, Chemistry of Biomolecules (2010), CRC Press
- 12. A. R. West Solid State Chemistry and its Applications, John Wiley (2001).

#### **CHEMISTRY PROJECT - I**

PAPER: CHEM 1004C

**Total Marks: 50 (Theory 35 + Internal Assessment 15)** 

Credit: 02

To be carried out under the guidance of an assigned faculty member of the Department. Area of research topics or any specific topic will be given to the student concern for preparation of literature report that to be submit for evaluation.

# **CHEMISTRY PROJECT - II**

PAPER: CHEM 1005C

**Total Marks: 100 (Theory 70 + Internal Assessment 30)** 

Credit: 04

To be carried out under the guidance of an assigned faculty member of the Department. **Project Report Submission and presentation (experimental / theoretical work)**