Scheme for 2 Year M.Sc. Programme in Chemistry (Under CBCS)
Central University of Kashmir

Semester I

CODE	COURSE	CREDITS
Core Courses (CC)		
CHM20-CC-101	Inorganic Chemistry-I	04
CHM20-CC-102	Organic Chemistry-I	04
CHM20-CC-103	Physical Chemistry-I	04
CHM20-CC-104	Laboratory course based on CHM20-101, 102 & 103	04
Discipline Specific Elective (DSE)-Any Two		
CHM20-DSE-101	Analytical Chemistry	02
CHM20-DSE-102	Mathematics for Chemists	02
CHM20-DSE-103	Symmetry & Group Theory	02
Skill Enhancement Course (SEC)		
CHM20-SEC-101	Basic Synthesis & Instrumentation	04
	Total Credits:	**24**

Scheme for 2 Year M.Sc. Programme in Chemistry (Under CBCS)
Central University of Kashmir

Semester II

CODE	COURSE	CREDITS
Core Courses (CC)		
CHM20-CC-201	Inorganic Chemistry-II	04
CHM20-CC-202	Organic Chemistry-II	04
CHM20-CC-203	Physical Chemistry-II	04
CHM20-CC-204	Laboratory course based on CHM20-201, 202 & 203	04
Discipline Specific Elective (DSE)-Any Two		
CHM20-DSE-201	Environmental Chemistry	02
CHM20-DSE-202	Surfactants & their Applications	02
CHM20-DSE-203	Asymmetric Synthesis, Advance Organic Reactions	02
	& Supramolecular Chemistry	02
Ability Enhancement Course		
CHM20-AEC-201	Quality Control & Quality Assurance	04
	Total Credits:	**24**

Scheme for 2 Year M.Sc. Programme in Chemistry (Under CBCS)
Central University of Kashmir

Semester III

CODE	COURSE	CREDITS
Core Courses (CC)		
CHM20-CC-301	Advanced Inorganic Chemistry	04
CHM20-CC-302	Advanced Organic Chemistry	04
CHM20-CC-303	Advanced Physical Chemistry	04
CHM20-CC-304	Laboratory course based on CHM20-301, 302 & 303	04
Discipline Specific Elective (DSE)-Any Two		
CHM20-DSE-301	Green Chemistry & Food Chemistry	02
CHM20-DSE-302	Medicinal Chemistry	02
CHM20-DSE-303	Non-equilibrium Thermodynamics & Quantum Chemistry	02
Open Generic Elective (OGE)		
CHM20-OGE-301	Chemistry & Life	04
	Total Credits:	**24**

Scheme for 2 Year M.Sc. Programme in Chemistry (Under CBCS)
Central University of Kashmir
Semester IV

CODE	COURSE	CREDITS
Specialization (Inorganic Chemistry)		
Core Courses (CC)		
CHM20-CC-401	Organo-Transition Metal Chemistry	04
CHM20-CC-402	Photo-Inorganic Chemistry	04
CHM20-CC-403	Advanced Laboratory Course in Inorganic Chemistry	04
Discipline Specific Elective (DSE)-Any one		
CHM20-DSE-401	Biological Inorganic Chemistry	02
CHM20-DSE-402	Non-Aqueous, Supramolecular & Inorganic Polymer Chemistry	02
Specialization (Organic Chemistry)		
Core Courses (CC)		
CHM20-CC-404	Chemistry of Natural Products	04
CHM20-CC-405	Reagents & Designing Organic Synthesis	04
CHM20-CC-406	Advanced Laboratory Course in Organic Chemistry	04
Discipline Specific Elective (DSE)-Any one		
CHM20-DSE-403	Basic Organic Reactions-The Biological Connection	02
CHM20-DSE-404	Heterocyclic Chemistry	02
Specialization (Physical Chemistry)		
Core Courses (CC)		
CHM20-CC-407	Advanced Quantum Chemistry	04
CHM20-CC-408	Statistical Mechanics & Advanced Electrochemistry	04
CHM20-CC-409	Advanced Laboratory Course in Physical Chemistry	04
Discipline Specific Elective (DSE)-Any one		
CHM20-DSE-405	Chemistry of Materials	02
CHM20-DSE-406	Advanced Photochemistry & Radiation Chemistry	02
Common Core Courses (CCC)		
CHM20-CC-410	Biochemistry & Chemical Biology	04
CHM20-CC-411	*$^{\#@}$Journal Club & **$^{\$@}$Seminar	02
CHM20-CC-412	$^{\$@}$Professional Development & Career Progression (National & International)	04
	Total Credits:	**24**

*Journal Club & **Seminar.

[#]Each student under the supervision of a Faculty/Advisor will present one original manuscript from a reputed Journal to the Department.
[$]Each student under the supervision of a Faculty/Advisor will present one Recent Review article(s) based seminar to the Department.
[@]Departmental Evaluation by Faculty, HOD & Dean, School of Physical & Chemical Sciences.

(Semester-I)

CHM20-CC-101 **Inorganic Chemistry-I**
Time: 60 Hours **Credits: 04**

Unit I: Bonding & Stereochemistry in Main Group Elements (15 Lectures)

Energy changes taking place during the formation of diatomic molecules; factors affecting the combined wave function. Bent's rule and energetics of hybridization. Resonance: Conditions, resonance energy and examples of some inorganic molecules/ions. Odd Electron Bonds: Types, properties and molecular orbital treatment. VSEPR: shapes of trigonal bipyramidal, octahedral and pentagonal bipyramidal molecules/ions. Limitations of VSEPR theory. Molecular orbital theory: Salient features, variation of electron density with internuclear distance. Relative order of energy levels and molecular orbital diagrams of some hetero-diatomic molecules/ions. Molecular orbital diagram of polyatomic molecules/ions. Delocalized Molecular Orbitals: Butadiene, cyclopentadiene and benzene. Hydrogen bonding: types and importance.

Unit II: Coordination Chemistry (15 Lectures)

Stepwise and overall formation constants, Mechanisms of complexation process (selected examples). Inert & labile complexes, d^n configuration and lability Stabilization of uncommon oxidation states in water. Metal Chelates: Chelate effect and the factors affecting stability of metal chelates (HSAB concept, Ligand preorganization, restricted rotation and pseudoaromaticity). Macrocycles(crown ethers, cryptands calixarenes). Applications of coordination compounds in medicine and analytical chemistry. Determination of formation constants by pH-metry and Spectrophotometry.

Unit III: Bonding in Coordination Compounds (15 Lectures)

Structural (ionic radii) and thermodynamic (hydration and lattice energies) effects of crystal field splitting. Jahn -Teller distortion. Experimental evidences in favor of Metal Ligand Orbital Overlap. Spectrochemical series and nephleuxetic effect. Angular overlap model. Molecular orbital theory of bonding in octahedral complexes: composition of ligand group orbitals; molecular orbitals and energy level diagram for sigma bonded ML_6; CFT applications from MOT, Effect of pi-bonding. Molecular orbital treatment and energy level diagram for bonding in Square-planar, Tetrahedral complexes and Ferrocene.

Unit IV: Pi-acid Metal Complexes (15 Lectures)

Transition Metal Carbonyls: EAN applications, Carbon monoxide as pi acceptor ligand, synthesis, reactions, structural diversity and bonding in mono and polynuclear carbonyls.IR, NMR) characterization of metal carbonyls for structural diagnosis. Cyanido complexes of d block metals. Toxicity of carbon monoxide and cyanide ligands. Preparation, structure and bonding modes of transition metal nitrosyls, dinitrogen, dioxygen and dihydrogen complexes. Tertiary phosphine as pi acceptor ligand, substituent effects on the ligand character of phosphine (cone angles).

Books Recommended:

1. Principles of Inorganic Chemistry; 1st edn.; Brain W. Pfennig; Wiley; 2015.

2. Advanced Inorganic Chemistry; 5th. and 6th edn; F.A. Cotton, G. Wilkinson; Wiley; 1998/1999.
3. Inorganic Chemistry; 4th edn; J. E. Huheey; E. A. Keiter; Harper Collins; 2009.
4. Chemistry of the Elements; 2nd edn; N. N. Greenwood, A. Earnshaw; Butterworth; 1997.
6. Inorganic Chemistry; 3rd edn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
7. Inorganic Chemistry; K.F. Purcell, J.C Kotz; Saunders; 1977.
8. Coordination Chemistry; D. Banerjea; Tata McGraw Hill; 1993
9. Chemistry of the elements, N.N. Greenwood and A. Earnshaw,2nd Edn. Pergamon
10. Wulfsberg, G. (1991). Principles of descriptive inorganic chemistry. University Science Books.
11. Housecraft, C. E., & Sharpe, A. G. Inorganic Chemistry, 4th Edn. 2012

CHM20-CC-102 **Organic Chemistry-I**
Time: 60 Hours **Credits: 04**

Unit I: Basic Concepts in Organic Chemistry (15 Lectures)

Electronic effects: Inductive effect, bond polarization and Polarazibility. Conjugation and resonance, steric inhibition of resonance. Isovalent and sacrificial Hyperconjugations and various types of tautomerism.

Aromaticity: Huckel's rule and concept of Aromaticity, Antiaromaticity and Homoaromaticity. NMR and aromaticity. Annulenes, heteroannulenes and fullerenes (C-60).

Reactive intermediates: Generation, structure, fate and stability of carbocations, (classical and non-classical) carbanions, free radicals, carbenes, nitrenes and arynes. Stability and reactivity of bridge-head carbocations. Bredt's rule.

Determination of Reaction Mechanism: Methods of determination of reaction mechanism, identification of products, transition state/intermediate. Isotopic labeling. Stereochemical, thermodynamic and kinetic evidences.

Unit II: Stereochemistry (15 Lectures)

Chirality: Chirality due to chiral centre, chirotopicity and stereogenicity. Pseudoasymmetric (D/L and R/S) descriptor, threo/ erythro / meso and syn/anti nomenclature. Stereo axis: chiral axis in allenes & biphenyls, R/S descriptor: cis/trans, syn/anti, *E/Z* descriptors (at C=C and C=N bonds). Optical activity of chiral compounds: specific rotation, optical purity (enantiomeric excess), Enantiotopic and diastereotopic atoms groups and faces. Felkin-Anh and Cornforth model, Cram's and Prelog's rules.

Conformations: Origin of conformational energy, Angle and Pitzer strain, conformational analysis of cycloalkanes and decalins. Conformation of sugars (anomeric effect), cyclohexene, cyclohexanones and bicyclo heptane-a bridged system. Effect of conformation on reactivity: stereoelectronic effects.

Unit III: Mechanistic Study of Organic Reactions-I (15 Lectures)

Aliphatic Nucleophilic Substitution Reactions: Mechanism and stereochemical implications of S_N2, S_N1, S_Ni and neighbouring Group Participation by π and σ-bonds. Comparison of S_N1 and S_N2 reactions. Effect of substrate structure, nucleophile, leaving group and solvent on the rates of S_N1 and S_N2 reactions. Mixed S_N1 and S_N2 reactions. Nucleophilic substitution at allylic, benzylic, aliphatic trigonal and vinylic carbons. Nucleophilic substitution in alcohols (Mitsunobu reaction), ethers and epoxides.

Unit-IV: Mechanistic Study of Organic Reactions-II (15 Lectures)

Elimination Reactions: Factors affecting elimination reactions, Mechanism of E_1, E_2, E_1cB and E_2C reactions. Competition between substitution and elimination reactions. Stereochemistry and regioselectivity of E_2 eliminations. Elimination in cyclic systems and vinyl halides. Mechanism and orientation in pyrolytic eliminations, Shapiro reaction.

Aliphatic Electrophilic Substitutions: General mechanism of S_E1, S_E2 and S_Ei reactions. Mechanisms of reactions involving migration of double bond. Effect of substrate, leaving group and solvent on reactivity. Stork-enamine reaction.

Books Recommended:

1. Advanced Organic Chemistry Reactions, Mechanism and Structure; 6th edn; Jerry March; Wiley; 2014.
2. Advanced Organic Chemistry; 5th edn; F. A. Carey and R. J. Sundberg; Plenum; 2007.
3. A Guide Book to Mechanism in Organic Chemistry; 6th edn; Peter Sykes; Longman; 1996.
4. Reaction Mechanism in Organic Chemistry; 3rd edn; S.M. Mukherjee and S.P. Singh; Macmillan; 1998.
5. Stereochemistry of Organic Compounds; 2nd edn; D. Nasipuri; New Age Inter; 2008.
6. Stereochemistry of Carbon Compounds; E.L.Eliel; TMH; 2007.
7. Stereochemistry of Organic Compounds l'" Ed. - P.S. Kalsi. (New Age lnter.- 2012).
8. Fundamentals of Organic Chemistry; 10th edn; Solomons; Wiley; 2012.
9. Organic Chemistry - 2"o Ed., J. Hornbackf (Brooks/Cole- 2006,
10. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole-2000).
11. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2012)

Time: 60 Hours **Credits: 04**

Unit I: Equilibrium Thermodynamics (15 Lectures)

Overview of the laws of thermodynamics: Thermodynamic Equilibria and Free Energy Functions, Physical Equilibria Involving Phase Transitions, Thermodynamic Maxwell Relations.

Partial molar quantities: Partial molar free energy, Partial molar volume and Partial molar heat content and their significances. Determinations of the partial molar quantities. Chemical potential and other thermodynamic functions, Variation of chemical potential with temperature and pressure, Chemical potential for Ideal gas mixture, Thermodynamic Functions of Mixing, Concepts of Fugacity and its determination, Non-ideal systems: Excess functions for non-ideal solutions. Gibbs Duhem Margules equation and its applications.

Unit II: Chemical Kinetics-I (15 Lectures)

Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory. Theories of unimolecular reactions (Lindman, Hinshelwood, RRK and RRKM theories). General features of fast reactions, study of fast reactions by flow method, relaxation method and flash photolysis. Explosive reactions, Polymerization reactions (free radical, cationic and anionic).

Unit III: Electrochemistry (15 Lectures)

Electrified interface, concept of surface excess. Thermodynamics of electrified interface, Lipmann equation, electro capillary curves. Methods for determination of surface excess. Structural models of metal-electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern models. Ionic Adsorption at electrodes – isotherms for adsorption (Langmuir, Frumkin and Temkin isotherms). Electron transfer at electrified interface at and away from equilibrium. Derivation of Butller-Volmer equation, low and high field approximations. Introduction to corrosion - mechanism and types of corrosion, corrosion current and corrosion potential. Electrodics of corrosion in absence of oxide layer, monitoring of corrosion, and inhibiting corrosion.

Unit IV: Quantum Chemistry-I (15 Lectures)

Exact Quantum Mechanical Results: Time-independent and time-dependent Schrodinger equation. Postulates of quantum mechanics. Operator concept, quantum mechanical operators in Cartesian and Spherical polar co-ordinate systems, some properties of quantum mechanical operators. Review of particle in a box problem. The solution of problems of harmonic oscillator & the rigid rotator. Tunneling effect. Born-Oppenheimer approximation. Solution of the Hydrogen-like atom problem- radial and angular wave functions.

Books Recommended:

1. Physical Chemistry; P. W. Atkins; ELBS; Oxford; 1997.
2. Physical Chemistry-A Molecular Approach; D. A. McQuarie & J. D. Simon; University Science Books; 1997.
3. Modern Electrochemistry; 1, 2A, 2nd edn; J.O M. Bokris and A. K. Reddy; Kluwer Academic/Plenum Publishers; New York.
4. Molecular Thermodynamics, D. A. McQuarrie, J. D. Simon, USB, 1998.
5. Understanding non-equilibrium thermodynamics. G. Lebon, D. Jon, J. Casas-Vasques. Springer, 2008. 6. Non-equlibrium thermodynamics, 2nd ed. Yasar Demirel. Elsevier, 2007.
6. Molecular Thermodynamics of Electrolyte Solutions, Lioyd L Lee, World Scientific, 2008.
7. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
8. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.
9. Introduction to Quantum chemistry - A. K. Chandra, TataMcGraw Hill, 1997.
10. Quantum Chemistry - Ira. N. Levine, 7th Edition, Pearson, 2009.
11. Quantum Chemistry, R. K. Prasad, 2nd Edition, New Age Publishers, 2001.
12. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
13. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola, New York, 2001.
14. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989
15. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001

CHM20-CC-104 **Laboratory course based on CHM20-101, 102 & 103**
Time: 180 Hours **Credits: 04**

Unit I: Basic Laboratory Course in Inorganic Chemistry

Theoretical appraisal of Inorganic laboratory techniques:

A Titrimetry:

Skill of titration and calculations. **Complexometric titrations:** Types of EDTA Titrations MetallochromicIndicators:Selection, structure, and mechanism of action. Role and selection of buffers in complexometric titrations,

Estimation of binary metal ion mixture using Gravimetry & Tritimetry simultaneously:

i) Silver (Ag+) as AgCl and Nickel (Ni^{2+}) as $[NiEDTA]^{2-}$ complex.

ii) Barium (Ba^{2+}) as $BaSO_4$ and Zinc as $[ZnEDTA]^{2-}$ complex.

v) Copper (Cu^{2+}) as CuSCN and Magnesium (Mg^{2+}) as $[MgEDTA]^{2-}$ complex.

B. Preparation of the following compounds:

i) $[Cu\ (acac)_2].2H_2O$

ii) Cis- $K[Cr(C_2O_4)_2(H_2O)]_2$

iii) $K_3[Fe(C_2O_4)_3].3H_2O$

Unit II: Laboratory Course in Organic Chemistry

A. Purification techniques (Demonstrations). Purification of solvents and reagents using techniques like crystallization, sublimation, fractional distillation, vacuum distillation, drying and storage of solvents, thin layer chromatography and column chromatography etc.

B. Preparations

1.1. Beckman rearrangement starting from acetophenone.

1.2. Haloform reaction: Preparation of Iodoform

1.3. Aromatic electrophillic substitutions inbenzene, benzoic acid or aniline.

C. Identification of Single Organic Compounds using physico-chemical properties.

Unit III: Laboratory Course in Physical Chemistry

A. *Chemical Kinetics:*

1. Study of kinetics of hydrolysis of an ester catalyzed by Dil. HCl.

2. Determination of order of reaction between $K_2S_2O_8$ and KI by Initial rates method.

B. *Viscometry:*

1. Investigation of variation of viscosity with conc. and determination of unknown concentration.

2. Estimation of molecular radius of a solute using viscometry.

C. Calorimetery

1. Determination of heat of neutralization of a strong acid and weak acid with a strong base.

Books Recommended:

1. Vogel's Textbook of Quantitative Chemical Analysis; 5th edn; Jeffery, Bassett; ELBS; 1989.
2. Quantitative Analysis; 6th edn; Day, Underwood; Printice Hall; 1993.
3. Analytical Chemistry; 6th edn; D. Christian; Wiley; 2008.
4. Microscale and Macroscale Organic Experiments; K.L. Williamson; D.C. Heath and Co; 1989.
5. Advanced Practical Organic Chemistry; 2nd edn; N.K. Vishnoi; Vikas; 1999.
6. Vogel's Textbook of Quantitative chemical Analysis; 5th edn; Jeffery, Bassett; ELBS; 1989.
7. Practical Physical Chemistry; Findley, Kitchener; Longman; 1977.
8. Advanced Practical Physical Chemistry; Yadav; Goel Pub; 1994.
9. Experiments in Physical Chemistry; 5th edn; Schoemaker et al MGH; 1989.

CHM20-DSE-101 **Analytical Chemistry**
Time: 30 Hours **Credits: 02**

Unit I: Scope & Objectives (07 Lectures)

Introduction: Analytical chemistry and chemical analysis, Classification of analytical methods, Method selection, Sample processing, Steps in a quantitative analysis, Quantitative range (bispartite classification), Data organization, Analytical validations, Limit of detection and limit of quantitation, The tools of analytical chemistry and good lab practices.

Unit II: Analytical Chemometrics (08 Lectures)

Propagation of measurement uncertainties (inaccuracy and imprecision). Useful statistical test: test of significance, the F test, the student‘t’ test, the chi-test, the correlation coefficient,

confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation. Chemometrics for optimization, modeling and parameter estimation, factor analysis, resolution and pattern recognition.

Unit III: Chromatographic Methods (07 Lectures)

Principle of chromatography, Classifications of chromatography, Brief idea about the techniques of planar and column chromatography, Gas chromatography and High-performance liquid chromatography.

Unit IV: Electromeric Methods (08 Lectures)

Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods

Books Recommended:

1. D.A. Skoog, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College Publishing, Philadelphia, London.
2. G.W. Ewing, Instrumental Methods of Chemical Analysis, 5th Edition (1978), McGraw Hill Books Co., New York.
3. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
4. J.H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt, London.
5. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
6. G. D. Christian, Analytical Chemistry, 5th Edition (1994), John Wiley & Sons, New York.
7. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Analytical Chemistry - An Introduction, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.
8. J. H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt,

CHM20-DSE-102 Mathematics for Chemists
Time: 30 Hours Credits: 02

Unit I: Determinants & Matrix Algebra (07 Lectures)

Determinants: Basic concepts, types and properties, Solution of equations by using Determinants.

Matrices: Types of matrices, transpose, adjoint & inverse of matrices, symmetric, skew-symmetric, hermitian, skew-hermitian, unitary matrices, trace of a matrix; Inverse of a matrix ,Solution of equations by matrix method, Characteristic equation of a matrix and its solution, Callay-Hamilton theorem (statement only).

Unit II: Calculus (Differentiation & Integration) (08 Lectures)

Differential Calculus: Limit, continuity and differentiability of a function. Rules for differentiation, maxima and minima, applications (Maximally populated rotational levels, Bohr's radius, most probable velocity from Maxwell distribution and applications to

thermodynamic properties). Partial differentiation, Euler's theorem (statement only) and its applications.
Integral calculus and Fourier series:Integration, basic rules for integration, integration by substitution, by parts, partial fractions. Fourier series and some simple applications/problems.

Unit III: Elementary Differential Equations (07 Lectures)
Variables-separable, homogeneous, linear equation, Bernoulli's equations, exact differential equation, second order differential equations and their solutions. (Applications to chemical kinetics and quantum chemistry.)

Unit IV: Probability & Vectors (08 Lectures)
Probability: Binomial theorem (statement only) and its simple applications, Permutations and Combinations, Mathematical Probability: Sample Space, Events. Simple problems on probability. Probability distribution function,discrete and continuous, Simple problems on probability distribution including binomial and Poisson distribution.
Vectors: Basic definitions Scalar, Vector and triple products with applications. Gradient, divergence and curl of a vector.

Books Recommended:

1. Physical Chemistry; Thomas Engel & Philip Reid; Pearson Education;
2. The Chemistry Mathematics Book; E. Steiner; Oxford;
3. Mathematics for Chemistry; G. Doggett & B.T. Sutcliffe; Longmann; 1995.
4. Mathematics for Physical Chemistry; R. G. Mortimer; Esevier; 2005.
5. Mathematical Methods for Scientists and Engineers; D.A.McQuarie; University Science Books; 2003.
6. Chemical Mathematics; D. M. Hirst; Longman.
7. Basic Mathematics for Chemists; Tebbutt; Wiley.
8. Mathematics for Chemists; C. L. Perrin; Wiley; 1970.

CHM20-DSE-103 Symmetry & Group Theory
Time: 30 Hours Credits: 02

Unit I: Molecular Symmetry-I (08 Lectures)
Molecular Symmetry: significance to chemical behavior, symmetry elements and operations: Identity, rotation axis, reflection plane, inversion centre, improper rotation axis. Combination of symmetry operations. Systematic procedure for assignment of point groups to molecules (Hands on/ exercises).

Unit II: Molecular Symmetry-II (07 Lectures)
Symmetry classes and their geometrical significance. Symmetry Groups, subgroups, and group multiplication tables. Point groups. Schoenflies notation of point groups. Matrices and their combination, block factored matrices, Matrix representation of symmetry operations.

Unit III: Symmetry & Group Theory (08 Lectures)

The Great Orthogonality theorem (elementary idea), consequences of the Great Orthogonality theorem. Reducible and Irreducible representations, character of a representation, properties of irreducible representations, Mullikan symbols for IRS. Character table: construction of character tables for C2v, C3v and C4v point groups.

Unit IV: Symmetry & Spectroscopy (07 Lectures)

Applications of group theory to IR and Raman spectroscopy, Symmetry of IR and Ramanactive normal vibrational modes of AB_2, AB_3, AB_4, AB_5, and AB_6 type molecules. Applications of symmetry to Molecular Chirality, Fluxionality and Polarity.

Books Recommended:

1. Chemical Applications of Group Theory; 2nd edn. F.A.Cotton; Wiley Eastern; 1994)
2. Molecular Symmetry and Group Theory; L. Carter; Wiley; 1998.
3. Symmetry and Spectroscopy of Molecules; K. Veera Reddy; New Age 1998.
4. Inorganic Chemistry, Principles of structure and reactivity; 4th Edition; James E. Huheey, Ellen A. Keiter and Richard L. Keiter. Pearson Education Inc.
5. Chemistry of the elements, N.N. Greenwood and A. Earnshaw, 2nd Edn. Pergamon
6. Housecraft, C. E., & Sharpe, A. G. Inorganic Chemistry, 4th Edn. 2012

CHM20-SEC-101 **Basic Synthesis & Instrumentation**

Time: 60 Hours **Credits: 04**

Unit I: Organic Synthetic Methods-I (15 Lectures)

Introduction to synthesis, strategy of synthesis, Retrosynthesis. Designing of green synthesis: choice of starting materials, reagents, catalysts and solvents. Basic principles of green chemistry and synthesis of organic compounds involving basic principles of green chemistry methodology of synthesis.

Unit II: **Organic Synthetic Methods-II (15 Lectures)**

Mechanism of reaction for synthesis of important organic compounds, new methods in organic synthesis: microwave technique, use of phase transfer catalyst in organic synthesis. Functional group exchange reactions. Oxidation. Reduction. Hydroboration. Protecting Groups. Stereo-control.

Unit III: Instrumental Methods of Chemical Analysis (15 Lectures)

Basic theory, instrumentation, laboratory techniques and analytical application of the following: Absorption Spectrophotometry: UV-visible, Fourier Transform Infrared Spectroscopy, Nuclear Magnetic Resonance, Electron Spin Resonance, Mass Spectrometry.

Unit IV: Chromatographic & Spectroscopic Techniques (15 Lectures)

Chromatography: Adsorption, Ion-exchange and High Pressure Liquid Chromatography. Atomic Absorption Spectroscopy, Emission Spectrophotometry: Induction Coupled Plasma Emission Spectroscopy, X-Ray Photoelectron Spectroscopy.

Books recommended:

1. Skoog, West, and Harris: Analytical Chemistry: an Introduction Saunders, College Publishing, 7th Edition
2. Skoog, Holler and Nieman: Principles of Instrumental Analysis, Fifth Edition, Brooks/Cole Thompson Learning Publishers.
3. Vogel's Quantitative Chemical Analysis, 6th Edition.
4. Kenneth A. Rubinson: Contemporary Instrumental Analysis, Culinary and Hospitality Industry Publications Services.
5. Allen J. Bard, Larry R. Faulkner: Electrochemical Methods: Fundamentals and Applications, 2nd Edition.
6. P.T. Anastas, J.C. Warner: Green Chemistry: Theory and Practice. Oxford University Press.
7. C. M. Starks and M Halpen: Phase Transfer Catalysts Chapman and Hall, NY.
8. V.K. Ahaluwalia and R. Agrawal: Organic Synthesis: Special Techniques. Narosa Publishing House, New Delhi.
9. Introduction to Modern Liquid Chromatography, Lloyd R. Snyder, Joseph J. Kirkland, John W. Dolan, 2009.
10. Practical High-Performance Liquid Chromatography, Veronika R. Meyer, |2010.
11. Liquid Chromatography Time-of-Flight Mass Spectrometry: Principles, Tools, and Applications for Accurate Mass Analysis, Imma Ferrer, E. Michael Thurman, 2009.

Syllabus for 2 Year M.Sc. Programme in Chemistry (Under CBCS)
(Semester-II)

CHM20-CC-201 **Inorganic Chemistry-II**
Time: 60 hours **Credits: 04**

Unit I: Basic Organometallic Chemistry (15 Lectures)

Importance of organometallic compounds as reagents, additives and catalysts. Nomenclature and classification of organometallic compounds. Comparisons of main group and transition metal organometallics. Effective atomic number rule and its utility in organometallics. Stability of organometallic compounds towards heat, oxidation and hydrolysis. Preparation, structure and bonding of Alkyls and aryls of Li, B and Al. Synthesis, Structure and bonding in Zeise's Salt. Homogenous Catalysis: Terminology, Tolman Catalytic loop; Mechanism of Hydrogenation and Hydroformation reactions in alkenes.

Unit II: Mechanism of Ligand Substitution Reactions in Octahedral Metal Complexes (15 Lectures)

Energy profile of a reaction; reactivity of metal complexes; inert and labile complexes. Types of substitution reactions; mechanistic classification of substitution reactions:-Dissociative, Associative, Dissociative conjugate base and Interchange. Empirical criteria to differentiate the mechanism of substitution. Substitution in octahedral complexes- Classification of metal ions based on water exchange rates. Metal-complex formation- the Eigen-Wilkins mechanism. Anation reactions. Hydrolysis Reactions; Simple Acid hydrolysis, Acid catalyzed and Base hydrolysis. Stereochemical changes in Octahedral Substitution Reactions. Substitution reactions without metal-ligand bond breaking.

Unit III: Mechanism of Ligand Substitution Reactions in Square-Planar complexes

(15 Lectures)

Significance of the two-term rate law, Mechanism, and Steric course of the substitution reactions. Factors affecting the rate of substitution: Entering and leaving groups; nucleophilicity of entering group and the npt scale, central metal ion, solvent, and the non-leaving groups. The Trans effect: Theories, applications in synthesis. Cis-trans isomerization in square planar complexes.

Unit IV: Electron Transfer Reactions in Coordination Complexes (15 Lectures)

Complementary and non-complementary reactions. Characterization of redox reactions as outer and inner sphere. Mechanism of outer sphere and inner sphere electron transfer reactions, rate laws. Factors affecting the rate of electron transfer- Chemical activation; sigma and pi nature of donor/ acceptor orbitals; Electron configuration of oxidant/reductant. Bridging ligand effects in inner sphere reactions. Differentiation of inner sphere and outer sphere electron transfer reactions. Electron transfer reaction in metalloproteins (Elementary idea). Oxidative addition, reductive elimination and migration (insertion) reactions.

Books Recommended:

1. Advanced Inorganic Chemistry, 6th ed. /5th ed. F.A. Cotton, G. Wilkinson (Wiley 1999/1988).
2. Inorganic Chemistry, 4th ed. J. E. Huheey, E. A. Keiter (Harper Collins, 1993).
3. Chemistry of the Elements 2nd ed. - N. N. Greenwood, A. Earnshaw (Butterworth, 1997).
4. Mechanisms of Inorganic Reactions - D. Katakis, G. Gordon (Wiley, 1987).
5. Reaction Mechanism of Inorganic and Organometallic systems, 2nd ed.- R. B. Jordan (Oxford, 1998).
6. Mechanisms of Inorganic Reactions, 2nd ed. - F. Basolo, R.G. Pearson (Wiley, 1967)
7. Inorganic Chemistry- K. F. Purcell, 1C. Kotz (Saunders, 1977).
8. Chemistry of the elements, N.N. Greenwood and A. Earnshaw, 2nd Edn. Pergamon
9. Wulfsberg, G. Principles of descriptive inorganic chemistry. University Science Books.
10. Housecraft, C. E., & Sharpe, A. G. Inorganic Chemistry, 4th Edn. 2012.

CHM20-CC-202 Organic Chemistry-II

Time: 60 Hours Credits: 04

Unit I: Mechanistic Study of Organic Reactions-III (15 Lectures)

Electrophilic Aromatic Substitution: Arenium ion mechanism, Sigma and pi – complexes, Energy profile diagram, Effect of leaving group. Orientation and reactivity in mono substituted benzene ring, *Ortho / Para ratio*, Ipso attack. The Third substitution: Orientation of substitution in benzene ring with more than one substituent. Orientation in other ring systems. Carboxylation of aromatic rings with $COCl_2$ and amidation with NH_2COCl. Reversal of F.C. acylations. Synthetic application of F.C. acylation and nitration reactions (Toluene to nitro-benzoic acids, synthesis of *ortho & Para* nitro anilines).

Nucleophilic Aromatic Substitution:Discussion of different nucleophilic aromatic substitution mechanisms (S_N1, S_NAr, Benzyne and $S_{RN}1$). Structure reactivity relationships. Effect of

leaving group and attacking nucleophile. Mechanisms of Von-Richter, Sommelet-Hauser and Smiles rearrangements and Chichibabin reaction.
Free radical Substitution: Mechanisms at an aromatic substrate. Neighbouring Group. Assistance in free radical reaction, reactivity for aliphatic and aromatic substrates. Reactivity in the attacking radical. Effect of solvent on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Free radical rearrangement and Hunsdiecker reaction.

Unit II: Mechanistic Study of Organic Reactions-IV (15 Lectures)

Addition to Carbonyl Bonds: Molecular orbital explanation of reactivity carbonyl group.
Mechanism of formation of cyano hydrins, hydrates, hemi-acetals, acetals, thio-acetals, imines, N-amines, oxines and hydrazones.
Replacement of carbonyl oxygen by hydrogen, addition of hydrides and organometallics.
Mechanism of Mannich, Aldol (Mukaiyama Aldol), Knoevenagel, Robinson annulation, Claisen, Dickman, Perkin, Stobbes, Darzens and Witting reaction.
Addition to carbon-carbon multiple bonds: General mechanism, reactivity, orientation and stereochemical implications of additions reactions involving electrophiles, nucleophiles and free radicals. Addition to cyclopropane ring. Hydrogenation of double/triple bonds and aromatic rings. Hydroboration, Ene-reaction. 1,2 and 1,4-addition of 1,3-dienes and Michael addition.

Unit III: Mechanistic Study of Organic Reactions-IV (15 Lectures)

Molecular Rearrangements: General mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements. Nature of migration and migratory aptitude and memory effect. Detailed study of following rearrangements: Ring expansion and contraction rearrangements, Wagner-Meerwein, Pinacol-Pinacolone, Semi-Pinacol, Demjanov, Benzil-Benzilic acid, Johnson orthoester rearrangement, Ireland-Claisen Rearrangement, Favorskii, Fries, Arndt-Eistert, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Pyne, homo-Pyne and Dienone-phenol rearrangements.

Unit IV: Pericyclic reactions (15 Lectures)

Molecular orbital symmetry, Frontier orbitals of ethene, 1,3- butadiene, 1,3,5-hexatriene and allylic systems. Different Approaches, HOMO, LUMO concept, FMO approach. Classification of Pericyclic reactions. Woodward Hofmann rules for the following pericyclic reactions.
Electrocyclic Reactions: Thermal and Photo-induced Electrocyclic reactions of 4n and 4n + 2 systems and their stereochemistry. Conrotatory and disrotatory motions
Cycloadditions: Thermal and Photochemical 2+2 and 4+2 cycloadditions. Suprafacial and antrafacial cycloaddition. Diels Alder reaction, Hetero-Diels Alder and inverse electron demand Diel's Alder reaction (IEDDAR).
Sigmatropic rearrangements: Classification, [1,3], [1,5] and [3,3] sigmatropic shifts. Claisen, Cope and oxy-Cope rearrangements. Suprafacial and antrafacial shifts of hydrogen atom. Problems based on of pericyclic reactions.

Books Recommended:

1. Advanced Organic Chemistry Reactions, Mechanism and Structure; 6th edn; Jerry March; Wiley; 2014.
2. Advanced Organic Chemistry 4th Ed. - F. A. Carey and R. J. Sundberg. (Plenum, 2001).
3. A Guide Book to Mechanism in Organic Chemistry 6th Ed.- Peter Sykes. (Longman, 1996).
4. Reaction Mechanism in Organic Chemistry 3rd Ed. - S.M. Mukherjee and S.P. Singh. Macmillan, 1998).
5. Fundamentals of Organic Chemistry , 5th ed.- Solomons. (Wiley, 1992)
6. Organic Chemistry, 5th Ed.- John McMurry. (Brooks/Cole, 2000)
7. Carruthers, W. and Coldham, I. Modern methods of organic synthesis, Cambridge University Press(2004).
8. Fleming, I. Pericyclic reactions, Oxford science publication (1998).
9. Photochemistry and pericyclic reactions by Jagdamba Singh and Jaya Singh, New Academic Science, 2009.
10. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2012).

CHM20-CC-203 **Physical Chemistry-II**
Time: 60 Hours **Credits: 04**

Unit I: Statistical Thermodynamics (15 Lectures)

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. Derivation of Boltzmann distribution law. Bose-Einstein and Fermi-Dirac distribution equations (without derivation) and comparison of the three statistics.

Partition function & its significance. Translational, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properties in terms of partition functions, application to ideal monoatomic & diatomic gases. Equilibrium constant in terms of partition functions.

Unit II: Solid State: Structure & Crystal Defects (15 Lectures)

Crystalline and Amorphous Solid, Unit cell, crystal lattices, Reciprocal lattice, Lattice planes, Miller indices; Bragg equation, Debye-Scherrer method of X-ray structural analysis of crystals, identification of cubic unit cells from systematic absences in diffraction pattern. *S*tructure factor and its relation to intensity and electron density.

Perfect and imperfect crystals, Intrinsic and extrinsic defects- point defects, line defectsand plane defects, Schottky and Frenkel defects, Thermodynamics of Schottky andFrenkel defect formation, Colour Centers,

Unit III: Properties of Solids (15 Lectures)

Free electron theory of metals: The Drude Model, Lorentz modification, Somerfield Model; Fermi-Dirac distribution function, Density of states.

(a) Electric Properties: Origin of bands, E-k diagrams, Bonding in solids, Band theory Semiconductors: Intrinsic and extrinsic semiconductors; p-n junction. Introduction, properties and applications of Superconductors.

(b) Dielectric Properties: Dielectric materials, Dielectric properties (dielectric constantand dielectric loss), Dependence of dielectric properties on size, Polarazibility, Conceptsof ferroelectricity, Pyroelectricity and Piezoelectricity.

(c) Magnetic Properties: Classification of materials on the basis of magnetic response, Effect oftemperature, Magnetic moment calculations, Ferro- and antiferromagnetic ordering,Dependence of magnetic properties on size, Magnetic domains and Hysteresis.

Unit IV:Surface Chemistry (15 Lectures)

Liquid Surface: Surface tension, pressure difference across curved surfaces (Laplace equation), vapor pressure of droplets (Kelvin equation), and Capillary condensation.

Solid liquid interface: Contact angle, young's equation, wetting, Wetting as contact angle phenomena. Thermodynamics of Interfaces: surface excess, surface tension and thermodynamic parameters, Gibbs adsorption isotherm. Solid surfaces: Adsorption at solid surfaces, adsorption models; Langmuir adsorption isotherm, BET adsorption isotherm and its use in estimation of surface area. Fumkin and Temkin adsorption equations. Adsorption on porous solids.

Books Recommended:

1. An Introduction to Chemical Thermodynamics, R. P. Rastogi and R. R. Mishra, VikasPublishing House Pvt. Ltd.
2. Statistical Thermodynamics (Hardback) By (author) M.C. Gupta, Publisher: New AgeInternational.
3. Thermodynamics, J. Rajaram and J.C. Kuriacose, Educational Publishers.
4. Physical Chemistry - P. W. Atkins, ELBS , Oxford, 1997.
5. Physical Chemistry- A Molecular Approach - D. A. McQuarie & J. D. Simon, University Science Books, 1997.
6. Introduction to Solids, Azaroff, Tata McGraw,1993.
7. Solid State Chemistry and its Applications, West, Wiley,1989.
8. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
9. Solid State Reactions, Schmalzried, Academic press, 1995.
10. Solid State Physics, N.W.Ashcroft and N.D.Mermin, Saunders college, 2001.
11. Elements of Solid state Physics, J.P. Srivastava, Prentice Hall of India, 2003.
12. Introduction to Colloid and Surface Chemistry 2nd Ed., D. J. Shaw, Butterworths,1970
13. Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast, 6th Edition, John Wiley and Sons, Inc. 1997.

CHM20-CC-204 Laboratory course based on CHM20-201, 202 & 203
Time: 180 Hours Credits: 04

Unit I: Laboratory Course in Inorganic Chemistry

A. Paper Chromatography of binary and ternary metal ion mixtures of first series transition metal ions (Co^{2+}, Ni^{2+} Cu^{2+}):

(i) Separation process, Technique of Paper Chromatography. Design of mobile phase.

(ii) Methods of paper chromatography (Ascending, Descending and Radial)

(iii) Comparative mobile phase study of separating mixtures. Chromatogram analysis.

B.Preparation of Transition metals Coordination compounds:

1. Synthesis as a Laboratory Technique: Calculations & Design of synthetic procedures.

Selected preparations of the coordination compounds with the specific objectives:

i) Mercurytetrathiocyanatocobaltate(II) : To visualize the complexation process.

ii) Tristhioureacopper(I)sulphate monohydrate : Stabilization of unusual oxidation state.

iii) Hexaamminecobalt(III) chloride : Multistep synthetic procedure

iv) Trisethylenediaminecobalt(III) chloride: Aerial oxidation racemic mixture resolution

Unit II: Laboratory Course in Organic Chemistry

A. Determination of Iodine, ester, acid and saponification values of an oil sample.

B. Organic Preparations

(a) Acetylation of Cholesterol or salicylic acid.

(b) Oxidation of Cyclohexanol by chromic acid to get adipic acid.

(c) Aldol condensation: Dibenzal acetone and benzaldehyde.

(d) Cannizarro's reaction of 4-Chlorobenzaldelyde.

(e) Diels Alder reaction between Benzoquinone and cyclopentadiene.

Unit III: Laboratory Course in Physical Chemistry

A.Determination of solubility and solubility product of sparingly soluble salt conductometrically.

B. Potentiometric titration of a redox system (ferrous ammonium sulfate with $K_2Cr_2O_7$).

C. Adsorption of acetic acid on charcoal to verify Freundlich adsorption isotherm*via* acid base titration.

D. Study of the kinetics of the iodination of acetone in the presence of acid by the initial ratemethod.

E. Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.

F. Determination of the rate constant of inversion of cane sugar catalyzed be HCl using polarimeter.

Books Recommended:

1. Vogel's Textbook of Quantitative Chemical Analysis; 5th edn; Jeffery, Bassett; ELBS; 1989.

2. Quantitative Analysis; 6th edn; Day, Underwood; Printice Hall; 1993.

3. Analytical Chemistry; 6th edn; D. Christian; Wiley; 2008.

4. Microscale and Macroscale Organic Experiments; K.L. Williamson; D.C. Heath and Co; 1989.

5. Advanced Practical Organic Chemistry; 2nd edn; N.K. Vishnoi; Vikas; 1999.

6. Vogel's Textbook of Quantitative chemical Analysis; 5th edn; Jeffery, Bassett; ELBS; 1989.

7. Practical Physical Chemistry; Findley, Kitchener; Longman;1977.

8. Advanced Practical Physical Chemistry; Yadav; Goel Pub; 1994.

9. Experiments in Physical Chemistry; 5th edn; Schoemaker et al MGH; 1989.

10. Experimental Physical Chemistry; Arthur M. Halpern, George C. McBane; Freeman; 2006.

CHM20-DSE-201 Environmental Chemistry

Time: 30 Hours **Credits: 02**

Unit I: Environment & Soil Chemistry (07 Lectures)

Introduction, Segments of Environment; Factors affecting environment. Biogeochemical process. Nature and Composition of Soil: Soil forming processes (pedogenesis) types of soil, soil profile, air, water, macro and micronutrients in soil. (clays, inorganic ions, organic matter and humus). Soil leaching, calcification and soil solution. Soil productivity evaluation (nitrogen, phosphorus and potassium). Acid—Base and Ion exchange as major chemical reactions in soil. Thermodynamics and kinetic modeling of ion exchange in soil. Soil acidification and treatment. Soil Pollution by Fertilizers, Pesticides, Plastics and Metals.

Unit II: Hydrosphere (08 Lectures)

Chemical Composition of Water Bodies: Factors determining composition (thermal stratification, acid-base, pE concept).Pourbiax and Distribution diagrams. Aquatic pollution: Inorganic, Organic, Agricultural, Industrial and Sewage. ***Water quality parameters:*** Dissolved oxygen, Metals, Content of Chloride, Phosphate, Nitrate, and Microorganisms. Water quality standards. ***Purification and treatment of water:*** Chlorination, Ozonation, UV radiation. Applications of Nanotechnology in water purification, advanced materials as water treatment catalysts.

Unit III: Atmosphere (07 Lectures)

Chemical Composition of the Atmosphere: Vertical profile of the atmosphere, Heat budget of earth's atmospheric system. Tropospheric reactivity patterns, Stratospheric Chemistry: Chapman cycle, ozone formation and mechanisms of ozone depletion by Chlorofluorocarbons. ***Greenhouse effect:*** Consequences and remedial measures. ***Acid rain:*** Chemical aspects, adverse effects and control. Photochemical smog formation.

Unit IV: Environmental Monitoring (08 Lectures)

Analytical methods for measuring air pollutants: General aspects, Sampling and methods of analyses. Continuous monitoring instruments as analytical tools for real time monitoring of air pollutants (NDIR, GC-MS, Chemiluminescence and Spectrophotometry).
Water Analysis Methods: Classical, Spectrophotometry, Electrochemical methods and Ion Chromatography. Analytical methods for determining dissolved oxygen, BOD and COD.
Choice of methods for determining trace metals (As, Cd, Hg, Pb and Se).

Books Recommended:

1. Fundamentals of Soil Behaviour", Mitchell.J.K," John Wiley, New York, 199
2. Yong.R.N and Warkentin.B.P, "Introduction to Soil Behaviour", Macmillan, Limited, London, 1979.
3. Lambe.T.W and Whitman.R.V, "Soil Mechanics", John Wiley and Sons, New York, 1979.
4. Hesse.R.P, "A textbook of soil chemical Analysis", CBS publishers & distribution, shahdara, delhi, 1994.
5. Environmental Chemistry; 5th edn; Colin Baird; Freeman & Co; 2012.
6. Environmental Chemistry; 9th edn.S.E.Manahan; Lewis Publishers;2009.
7. Environmental Toxicology; Ed.Rose; Gordon & Breach Science Publishers.

8. Chemistry of the Environment; IInd edn.; T. G. Spiro and W. M. Stigliani; Prentice Hall; 2002.
9. Chemistry of the Environment; IInd Edn. R. A. Bailey; H. M. Clark; J. P. Ferris; S. Krause & R. L. Strong; Elsevier; 2005.

CHM20-DSE-202 **Surfactants & their Applications**
Time: 30 Hours **Credits: 02**

Unit I: Self-Assembly of Surfactants (07 Lectures)

Surfactants and Micelles: Classification of Surfactants, Solubility of Surfactants: Kraft temperature and cloud point, Micellization of surfactants: critical micelle concentration (cmc), aggregation number, counterion binding, factors affecting cmc in aqueous media. Thermodynamics of micellization: pseudophase model and mass action models. Structure and shape of micelles: geometrical consideration of chain packing, variation of micellar size and shape with surfactant concentration.

Unit II: Micellar Solubilization & Catalysis (08 Lectures)

Introduction, factors affecting micellar solubilization: nature of surfactant/solubilizate, effect of additive and temperature. Effect of solubilization on micellar structure, cloud point and cmc of surfactants. Solubilization of drugs into micelles and its importance in drug delivery systems and controlled release. Theoretical consideration of reactions in micellar media. Examples of micellar catalysis in C-C bond formation, hydrolysis, oxidation and reduction reactions.

Unit III:Micro & Nano-Emulsions (07 Lectures)

Micro-emulsion, types of emulsions, Preparation methods, Theories of emulsions:Interfacial theory, Solubilization and Thermodynamic theory.
Nano-emulsion:types, preparation methods, and theories (turbulence and cavitation).

Unit IV: Surfactant-Polymer Systems (08 Lectures)

Effect of polymers on aggregation behavior of surfactants and the factors governing their interaction. Phase behavior of polymer-surfactant mixtures. Characterization of polymer-surfactant systems by various techniques like viscosity, light scattering, spectroscopic and conductance measurements. Applications of surfactant-polymers systems.

Books Recommended:

1. Properties of Liquids and Solutions; J.N. Murell and E. H. Boucher; John Wiley & Sons Ltd; 1982.
2. Physical Chemistry; P.W. Atkins; ELBS; Oxford; 1994.
3. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York; 1986.
4. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
5. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.

6. Surfactants and polymers in aqueous solution; Jonsson, Lindmann, Homberg and Kronberg; John Wiley and sons; 1998.
7. Advances in Colloid and Polymer Science; B.K.Paul & S.P.Moulik, Current Science,Vol.80,p 990-,2001; Vol.78,p 99,1998.
8. Kale, Santosh Nemichand, and Sharada Laxman Deore. "Emulsion micro emulsion and nano emulsion: a review." Systematic Reviews in Pharmacy 8.1 (2017): 39.

CHM20-DSE-203 Asymmetric Synthesis, Advance Organic Reactions & Supramolecular Chemistry

Time: 30 Hours Credits: 02

Unit I: Asymmetric Synthesis-I (07 Lectures)

Introduction, Chiral pool. Chiral auxiliaries, Determination of enantiomeric and diasteromeric excess. Enantio-discrimination.

Optical and Kinetic resolution. Methods of asymmetric induction-chiral substrates, Chiral reagents and asymmetric catalysis. Catalytic asymmetric reduction of ketones, Enantioselective alkylation of aldehydes and ketones via chiral hydrazones. Asymmetric reduction using chiral trialkyl boranes of aldehydes and ketones.

Unit II: Asymmetric Synthesis-II (08 Lectures)

Catalytic asymmetric reduction of alkenes, Synthesis of L-alanine and L-dopa. Asymmetric epoxidation and dihydroxylation of alkenes. Asymmetric conjugate additions. Asymmetric hydroboration with diisopinocamphenylboranes. Asymmetric Diels-Alder and Aldol reaction (Evans aldol). Enzymes as catalysts.

Unit III: Advance Organic reactions (08 Lectures)

Palladium Catalyzed Cross Coupling Reactions*:* Negishi, Heck, Suzuki, Sonogoshira, Stille and Buchwald Hartig coupling. Mechanism and importance in natural product synthesis.

Olefination Reactions*:* Wittig, Peterson, Julia and Tebbe olefination.

Metathesis reactions and concept of CH-activation.

Elementary idea about N-heterocyclic carbine chemistry (NHC) Chemistry

Unit IV: Supramolecular Chemistry (07 Lectures

Concepts-Definition, Development and Classification. Binding Constants, Supramolecular interactions. Supramolecular Chemistry in Life -Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly. Cation Binding Hosts-Podand, Crown Ether, Cryptand, Spherand. Alkalides, Electrides, Calixarenes, Siderophores.

Books Recommended:

1. Designing Organic Synthesis, S. Warren; Wiley; 2013. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin; Verlage VCH;1986.
2. Carruthers, W. and Coldham, I. Modern methods of organic synthesis, Cambridge University Press(2004).

3. 4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 2007.
4. Organic Chemistry, 10th edn;. T. W. G. Solomons and Craig B. Fryhle ; Wiley-2012.
5. Organic Chemistry; Clayden, Greeves, Warren and Wothers ; Oxford University Press-2012.
6. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013.

CHM20-201-AEC **Quality Control & Quality Assurance**
Time 60 Hours **Credit: 04**

Unit I: Introduction & cGMP guidelines (15 Lectures)

Concept and evolution and scopes of Quality Control and Quality Assurance, Good Laboratory Practice, GMP, Overview of ICH Guidelines – QSEM, with special emphasis on Q-series guidelines. Good Laboratory Practices: Scope of GLP, Definitions, Quality assurance unit, protocol for conduct of nonclinical testing, control on animal house, report preparation and documentation. CPCSEA guidelines.

cGMP guidelines according to schedule M, USFDA (inclusive of CDER and CBER) and WHO covering: Organization and personnel responsibilities, training, hygiene and personal records, drug industry location, design, construction and plant lay out, maintenance, sanitation, environmental control, utilities and maintenance of sterile areas, control of contamination and good warehousing practice.

Unit II: Analysis (15 Lectures)

Analysis of raw materials, finished products, packaging materials, in process quality control (IPQC), Developing specification (ICH Q6 and Q3), purchase specifications and maintenance of stores for raw materials. In process quality control and finished products quality control for following dosage forms in Pharma industry according to Indian, US and British pharmacopoeias: tablets, capsules, ointments, suppositories, creams, parenterals, ophthalmic and surgical products (How to refer pharmacopoeias).

Unit III: Documentation (15 Lectures)

Three tier documentation, Policy, Procedures and Work instructions, and records (Formats), Basic principles- How to maintain, retention and retrieval etc. Standard operating procedures (How to write), Master Batch Record, Batch Manufacturing Record, Quality audit plan and reports. Specification and test procedures, Protocols and reports. Distribution records. Electronic data handling. Concepts of controlled and uncontrolled documents. Submission documents for regulators DMFs, as Common Technical Document and Electronic Common Technical Documentation (CTD, eCTD). Concept of regulated and non-regulated markets.

Unit IV: Manufacturing Operations & Controls (15 Lectures)

Sanitation of manufacturing premises, mix-ups and cross contamination, processing of intermediates and bulk products, packaging operations, IPQC, release of finished product, process deviations, charge-in of components, time limitations on production, drug product inspection, expiry date calculation, calculation of yields, production record review, change control, sterile products, aseptic process control, packaging, reprocessing, salvaging, handling

of waste and scrap disposal. Introduction, scope and importance of intellectual property rights. Concept of trade mark, copyright and patents.

Recommended Books:

1. Quality Assurance Guide by organization of Pharmaceutical Procedures of India, 3rd revised edition, Volume I & II, Mumbai, 1996.
2. Good Laboratory Practice Regulations, 2nd Edition, Sandy Weinberg Vol. 69, Marcel Dekker Series, 1995.
3. Quality Assurance of Pharmaceuticals- A compedium of Guide lines and Related materials Vol I & II, 2nd edition, WHO Publications, 1999.
4. How to Practice GMP's – P P Sharma, Vandana Publications, Agra, 1991.
5. The International Pharmacopoeia – vol I, II, III, IV & V – General Methods of Analysis and Quality specification for Pharmaceutical Substances, Excepients and Dosage forms, 3rd edition, WHO, Geneva, 2005.
6. Good laboratory Practice Regulations – Allen F. Hirsch, Volume 38, Marcel Dekker Series, 1989.
7. ICH guidelines, ISO 9000 and total quality management
8. The drugs and cosmetics act 1940 – Deshpande, Nilesh Gandhi, 4th edition, Susmit Publishers, 2006.
9. QA Manual – D.H. Shah, 1st edition, Business Horizons, 2000.
10. Good Manufacturing Practices for Pharmaceuticals a plan for total quality control – Sidney H. Willig, Vol. 52, 3rd edition, Marcel Dekker Series.
11. Steinborn L. GMP/ISO Quality Audit Manual for Healthcare Manufacturers and Their Suppliers, Sixth Edition, (Volume 1 – With Checklists and
12. Software Package). Taylor & Francis; 2003.
13. Sarker DK. Quality Systems and Controls for Pharmaceuticals. John Wiley & Sons; 2008.
14. Packaging of Pharmaceuticals.Schedule M and Schedule N

Syllabus for 2 Year M.Sc. Programme in Chemistry (Under CBCS)
(Semester-III)

CHM20-CC-301 **Advanced Inorganic Chemistry**
Time 60 Hours **Credit: 04**

Unit I: Magnetic & Electronic properties of Transition Metal Complexes

(15 Lectures)

Types of magnetic behaviour, magnetic susceptibility and magnetic moment. Methods of determining magnetic susceptibility, spin-only formula, L-S coupling, correlation of μs and μeff values, orbital contribution to magnetic moments. Applications of magnetic moment data

in investigation of nature of bonding and stereochemistry of first row transition metal complexes. High spin low spin crossover. Temperature independent paramagnetism, Exchange pathways of antiferromagnetism and ferromagnetism in metal complexes, anomalous magnetic moments.

Types of electronic transitions, theoretical aspects of d-d spectra, selection rules and their relaxations, spectral terms of d^1 - d^{10} metal ions. Spectroscopic ground states. Charge transfer spectra. Simple problems on assigning electronic spectral data and calculation of ligand-field parameters.

Unit III: Bonding models in Inorganic Chemistry (15 Lectures)

Classification and topology of Boron clusters, types of bonds, isolobal analogy, empirical rules for bonding in boron clusters, Selected examples of bonding in higher boranes and Carboranes. Bonding in Boron–Nitrogen Compounds (Borazine),Phosphorous–Nitrogen compounds (Cyclophosphazenes and phosphonitrillic halides),Sulphur-Nitrogen compounds (polythiazyls).Bonding in metal clusters (di and trinuclear), cotton rationale and quadruple bonding, selected examples of bonding in dinuclear metal clusters. Bonding in transition metal polymetallates.

Unit IV: Inner Transition metal Chemistry (15 Lectures)

Properties of*f*- orbitals. Atom and ion sizes (Lanthanide Contraction), coordination numbers and stability of lanthanide complexes. Selected coordination chemistry of Ln(III). Organometallic complexes of lanthanides (cyclopentadienyl and cyclo-octatetraenyl ligand) Spin-Orbital Coupling, Magnetic Properties of Ln(III) ions. Adiabatic Demagnetization. Electronic spectra, Luminescence spectra. Applications of Lanthanide complexes as sensory probes, lasers, NMR shift reagents and MRI contrast agents.Actinides: electronic configuration, oxidation states, electronic spectra and magnetic moments. Chemistry of Inorganic salts, coordination complexes and organometallic compounds of thorium and uranium.

Unit IV: Inorganic spectroscopy: NQR & Mossbauer Spectroscopy (15 Lectures)

NQR Spectroscopy: NQR isotopes, Nuclear quadruple moment; Electric field gradient; nuclear quadruple coupling Constant; Effect of applied magnetic field, Applications.

Mossbauer Spectroscopy: Basic principles, Spectral parameters such as isomer shift, quadrupole splitting and magnetic splitting, spectrum display. Application of the technique to the studies of (i) bonding and structure of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (ii) Sn^{2+} and Sn^{4+} compounds, nature of M-L bond, coordination number and structure, (iii) detection of oxidation state and in equivalent MB atoms.

Books Recommended:

1. Housecraft, C. E., & Sharpe, A. G. Inorganic Chemistry, 4th Edn. 2012.
2. Inorganic Chemistry, Principles of structure and reactivity; 4th edition; James E. Huheey, Ellen A. Keiter and Richard L. Keiter. Pearson Education Inc.
3. Chemistry of the elements, N.N. Greenwood and A. Earnshaw, 2nd Edn. Pergamon
4. Electronic Spectra of Transition Metal Complexes; D. Sutton; McGraw-Hill; 1968.
5. NMR, NQR, EPR, and Mossbauer Spectroscopy in Inorganic Chemistry; R. V. Parish; Ellis Horwood; 1990.
6. Structural Methods in Inorganic Chemistry; 2nd edn.; E. A. V. Ebsworth & D.W.H. Rankin; ELBS; 1991.
7. Spectroscopy in Inorganic Chemistry; Vol I & II; Rao, Ferraro; Academic Press; 1970.

CHM20-CC-302 **Advanced Organic Chemistry**
Time 60 Hours **Credit: 04**

Unit I: Photochemistry-I **(15 Lectures)**

Photochemical Reactions: Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states and their lifetimes. The fate of excited molecule. (Physical and chemical processes). Transfer of excitation energy: Sensitization and Quenching. Quantum yield. Types of photochemical reactions. Photochemistry of alkenes: Geometrical isomerizations, cyclisation and dimerization reactions. Photochemical reactions of 1,3-butadiene (excluding pericyclic reactions). Rearrangement of 1,4 and 1,5- dienes. Photochemistry of saturated carbonyl compounds: Norrish type-I and Norrish type-II processes, Paterno-Buchi reaction.

Unit II: Photochemistry –II **(15 Lectures)**

Photochemistry of unsaturated carbonyl compounds: Photochemical reactions of α,β-unsaturated carbonyl compounds.(H-Abstraction and isomerization to β,γ, -unsaturated carbonyl compounds). Photolysis of cyclic α,β - unsaturated ketones (dimerization and lumiketone rearrangement) and cyclohexadienones.

Photochemistry of Aromatic compounds: Photoinduced isomerizations of benzene and its alkyl derivatives. 1,2 ; 1,3 and 1,4-photoaddition reactions of benzene. Nucleophilic Photo substitution reactions in aromatic compounds. Photo Fries-rearrangement of aryl esters and anilides.

Miscellaneous Photochemical reaction: Photolysis of organic nitrites and their synthetic utility (Barton reaction). Photochemistry of vision, Singlet Oxygen Addition to olefins.

Unit III: UV, IR & Mass Spectroscopy **(15 Lectures)**

Ultraviolet spectroscopy: Absorption spectra of enones, dienes (homo and heteroannular) carbonyl compounds, aromatic and heteroaromatic compounds. Effect of conjugation on ultraviolet spectra, Woodward-Fieser rules, Kuhn's rule, application to conjugated polyenes.

Infra-red spectroscopy: The Infra-red region, Finger print region, Characteristic vibrational frequencies of hydrocarbons, alcohols, ethers, phenols, amines, aldehydes, ketones, acids, anhydrides, esters, lactones, amides and conjugated carbonyl compounds. Effect of hydrogen bonding on vibrational frequencies in IR spectra, Overtones, combination bands and Fermi resonance.

Mass Spectrometry: Introduction, Schematic diagram of mass spectrometry. The mass spectrum-Nitrogen Rule, Metastable Peak. Fragmentation pattern like Stevenson rule, initial ionization event, α-cleavage, inductive cleavage, two bond cleavage, Retro-Diels. Alder cleavage, Mc-Laffertey Rearrangements. Mass spectra of different group of different compounds.

Unit IV: ^{1}H & ^{13}C-Nuclear Magnetic Resonance Spectroscopy **(15 Lectures)**

Basic concepts, Mechanism of Measurements, Chemical shift values for various classes of compounds. Fourier Transform (FT), Techniques and advantages, Nuclear Overhouser Effect (NOE). One bond coupling, two bond coupling, three bond coupling, second order spectra A_2, AB, AX, AB_2, AX_2, A_2B_2. Proton exchange, deuterium exchange, Peak broadening exchange ^{13}Carbon-chemical shifts, proton coupled and decoupled spectra. Nuclear Overhouser Effect, Off-Resonance De-coupling, Basic concepts of DEPT-4, DEPT-90, DEPT-135.

Introduction to two-dimensional spectroscopy methods, COSY, NOSY and HETCOR technique, NOSY. Structure determination of organic compounds based on their spectral data (UV, IR, NMR and Mass Spectrometry). Problem based exercises.

Recommended Books:

1. Introductory Photochemistry; A. Cox and T. Kemp; McGraw Hill; 1971.
2. Organic Photochemistry; 2nd edn.; J. Coxon, and B.Halton; Cambridge University press; 1987.
3. Fundamentals of photochemistry; Rohtagi & Mukherjee; Wiley Eastern; 1992.
4. Spectroscopy of Organic Compounds; 6th edn.; P. S. Kalsi; New Age Publishers; 2006.
5. Spectrometric identification of Organic Compounds; 5th edn.; R. M. Silverstein, G.C.Bassler and T.C.Morill; John Wiley; 1991.
6. Introduction to NMR Spectroscopy; R. J. Abraham. J. Fisher and P. Loftus; Wiley; 1991.
7. Applications of absorption spectroscopy of Organic Compounds, J.R.Dyer (Prentice Hall-1991).
8. Spectroscopic Methods in organic Chemistry; D. H. Williams, I. Fleming; Tata McGraw Hill; 1988.

CHM20-CC-303 **Advanced Physical Chemistry**
Time 60 Hours **Credit: 04**

Unit I: Equilibrium Thermodynamics of Electrolytes (15 Lectures)

Ion solvent Interactions: Non-structural (Born) treatment and an introduction tostructural (Ion-dipole, Ion-quadruple) treatments of ion-solvent interactions.

Ion-Ion Interactions: Activity and activity co-efficient. Debye-Huckel theory of activitycoefficients of electrolyte solutions; derivation of Debye-Huckel limiting law, validity andextension to high concentrations; ion-pair formation-Bjerrum model.Conductance of electrolyte solutions: Mobility of ions, mobility and conductivity, Einsteinrelations, dependence of molar conductance on concentration, estimation of K and Λ^0forweak electrolytes, Theories of Conductance: Debye-Huckel-Onsager conductance equationand brief idea of its extension.

Unit II: Quantum Chemistry-II (15 Lectures)

General theory of angular momentum. Eigen functions and Eigen values of angular momentum operators. Ladder operators. Spin angular momentum, antisymmetry and Pauli's principle. Atomic term symbols, term separation of p^n and d^n configurations, spin-orbit coupling, Zeeman splitting.

Approximation methods: The Variation theorem, linear variation principle, application to hydrogen atom and helium atom. Perturbation method. Chemical Bonding: LCAO-MO approximation, H_2^+ molecular ion, brief introduction to H_2. Molecular term symbols. Valence bond treatment of hydrogen molecule, comparison of MO and VB methods in the light of hydrogen molecule.

Unit III:Chemical kinetics-II (15 Lectures)

Surface Reactions:Unimolecular & bimolecular surface reactions [Langmuir-Hinshelwood & Langnuir- Riedel mechanism], classical & statistical treatments.Reactions in solutions:Effect of solvent on reaction rates, Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions, effect of ionic strength. Enzyme catalyzed Reactions: Kinetics of enzyme catalyzed reactions, Effect of substrate concentration, temperature and pH. Enzyme inhibition.Structure Reactivity Relationships: Quadratic Free-Energy Relationships (QFER), Hammet and Taft relationships.

Unit IV: Molecular, Vibrational-Rotational & Raman Spectroscopy (15 Lectures)

Molecular spectroscopy: Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and / or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules.

Vibrational spectroscopy: Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones. Dissociation energies from vibrational data. Vibration-rotation spectra, P, Q and R branches. Nuclear spin effect. Symmetry of normal coordinates. Use of Group Theory in assignment of spectra and selection rules for simple molecules.

Raman spectroscopy: Stokes and anti-Stokes lines. Polarazibility ellipsoids. Rotational and vibrational Raman spectroscopy. Selection rules. Rule of Mutual Exclusion. Polarization of Raman lines.

Books Recommended:

1. Molecular Thermodynamics of Electrolyte Solutions, Lioyd L Lee, World Scientific, 2008.
2. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
3. Physical Chemistry; P. W. Atkins; ELBS; Oxford; 1997.
4. Physical Chemistry- A Molecular Approach; D. A. McQuarie & J. D. Simon; University Science Books; 1997.
5. Introduction to Quantum chemistry; A. K. Chandra; Tata McGraw Hill; 1997.
6. Quantum Chemistry - Ira. N. Levine, Prentice Hall, 2000.
7. Quantum Chemistry, Prasad, New Age Publishers, 2000.
8. Hollas. J. M. *Modern Spectroscopy* 4th Ed., John Wiley & Sons (2004).
9. Satyanarayana, D. N. Handbook of Molecular Spectroscopy: From radio waves to gamma rays,I.K. International Publishing House, New Delhi (2015).
10. Kakkar, R., *Atomic & Molecular Spectroscopy,* Cambridge University Press (2015).
11. Brand, J. C. D. & Speakman, J. C. *Molecular Structure: The Physical Approach* 2nd Ed., Edward Arnold: London (1975).
12. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
13. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola, New York, 2001.
14. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989

15. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001.

CHM20-CC-304 **Laboratory course based on CHM20-301, 302 & 303**
Time 180 Hours **Credit: 04**

Unit I: Laboratory Course in Inorganic Chemistry

A. Qualitative Analysis by Semi micro Technique: Analytical groups and Group reagents. Scales of Analysis, Chemistry involved in separation and identification of less familiar cations by semi micro analysis.

Identification of four less familiar cations from different analytical group combinations

(i) Group I and II A (ii) Group I, II A and II B (iii) Group IIA and II B (iv) Group I and Group III (v) Group II B and Group III (vi) Group III only.

B: Spectrophotometry: (2 Experiments)

• Determination of Fe (II) with 1,10-Phenanthroline.

• Spectrophotometric titration of Fe(II) vs. $KMnO_4$.

Unit II: Laboratory Course in Organic Chemistry

A. Separation of organic compounds from three component mixture and their identification using physico-chemical methods.

B. Identification of simple compounds using IR/NMR spectra.

C. Quantitative Estimation of the following:

(a) Carbohydrates

(b) Carboxylic acids

Unit-III: Laboratory Course in Physical Chemistry

A. *pH metery*

1. Titration of with a tribasic acid alkali to find its pKa values.
2. Determination of degree of hydrolysis of aniline hydrochloride.

B.Spe*ctrophotometry*

1. Determination of composition of a binary mixture of $K_2Cr_2O_7$ and $KMnO_4$ or Cobalt (II) and Nickel (II) ions.
2. Spectrophotometric titration of Fe(II) vs. $KMNO_4$.

C. *Potentiometry*

1. Titration of Fe (II) vs $K_2Cr_2O_7$ and determination of standard redox potential of Fe^{2+}/Fe^{3+}.
2. Determination of formation constant of Ag-NH_3 complex.

Books Recommended:

1. Vogel's Textbook of Quantitative chemical Analysis; 5th edn; Jeffery, Bassett; ELBS; 1989.
2. Analytical Chemistry; 6th edn; D. Christian; Wiley; 2008.
3. Essence of Chromatography; Colin. F. Poole; Elsevier.Inc;
4. Chromatographic methods; A. Braithwaite and F. J. Smith; 5th edn.; Kluwer Academic Publishers; 1999.
5. Chromatographic Methods; 3rd edn.; Stock & Rice; Chapman & Hall; 1980.
6. Experiments and Techniques in Organic Chemistry; D. Pasto, C. Johnson and M. Miller; Prentice-hall; 1992.
7. Microscale and Macroscale Organic Experiments; K .L. Williamson; D.C. Heath and Co.; 1989.
8. Advanced Practical Organic Chemistry; 2nd edn.; N. K. Vishnoi; Vikas; 1999.
9. Vogel's Textbook of Practical Organic Chemistry; 5th edn.; A. R. Tatchell; ELBS; 1996.
10. Comprehensive Practical Organic Chemistry; V. K. Ahluwalia and Renu Aggarwal; University Press; 2000.

11. Electrochemical methods, Fundamentals and Methods; A.J. Bard, L.R. Faulkner; Wiley; 1980.
12. Physical Electrochemistry- Fundamentals, Techniques and Applications; Eliezer Gileadi; Wiley-VCH; 2011.

CHM20-DSE-301 **Green Chemistry & Food Chemistry**
Time: 30 Hours **Credits:02**

Unit I: Green Chemistry-I **(08 Lectures)**
Introduction, Need for Green Chemistry and the role of chemists. Principles of Green Chemistry.
Tools of Green Chemistry: Selection of starting materials, Catalysts, Alternative Solvents, Appropriate reagents, Percentage atom utilization. Microwaves and Sonication.

Unit II: Green Chemistry-II **(07 Lectures)**
Green Solvents and Reaction conditions: Supracritical fluids, aqueous reaction conditions, immobilized Solvents and irradiative reaction conditions.
Examples of Green materials, reagents and some specific reactions.

Unit III: Chemistry of Food Colors & flavors **(08 Lectures)**
Introduction. Pigments in animal and plant tissues: Chlorophyll, Carotenoids, Anthocyanin's and other Phenols. Natural and artificial food colorants.
Definition of flavor. Classification of food flavors. Chemical components responsible for the following: Sweetness, Saltiness, Sourness, Bitterness, Astringency, Pungency, Meatiness and Fruitiness. Synthetic flavouring.

Unit III: Chemistry of Food Preservatives **(07 Lectures)**
Introduction. Basis of Food Preservation. Food additives: Sodium Chloride, Nitrites, Smoke, SO2, Benzoates and other Organic acids. Auto-oxidation and antioxidants. Modified atmosphere and vacuum packaging. Toxins of plant foods. Toxins of animal foods. Toxic agriculture residue Toxic metal residue. Toxins generated during heating and packaging of food. Environmental pollutants of food stuff.

Books Recommended:

1. Green Chemistry- Environment Friendly Alternatives; Rashmi Sangh & M. M Srivastava; Narosa; 2007.
2. Green Chemistry- An Introductory Text; IInd Edn.; Mike Lancaster; RSC; 2010.
3. Green Chemistry- Theory and Practice; P. T. Anastas and J. C. Warner; oxford; 2000.
4. Green Chemistry; Ist Edn.; Samuel Delvin; IVY Publishing House; 2008.
5. Green Chemistry- Environmentally Benign Reactions; V. K. Ahluwalia; Ane Books; 2006.
6. Food Chemistry; Owen R. Fennema; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
7. Food: The Chemistry of its components; T.P. Coultate; 3rd Ed.; RSC Paperbacks; 1996.
8. Food Preservatives; H.J. Russell and G. W. Gould; 2nd ed.; Springer International Edition; 2005.

CHM20-DSE-302 **Medicinal Chemistry**
Time: 30 Hours **Credits:02**

Unit I: Drug design **(07 Lectures)**

Introduction and classification of drugs, Concept of lead compound, lead modification, prodrugs and soft drugs, structure-activity relationship (SAR), Functional-activity relationship (FAR); factors affecting bioactivity, resonance, inductive effect, isosterism, bioisosterism, spatial considerations. Occupancy theory, rate theory, induced fit theory. Concepts of drug receptors. Preliminary report of Free-Wilson and Hansch analysis.

Unit II: Antibiotics & Cardiovascular Drugs **(08 Lectures)**

Cell wall biosynthesis from β-lactum rings, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of Penicillin G, Ampicillin, Tetracycline, Ciprofloxacin, Norfloxacin, Cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Synthesis of amylnitrate, sorbitrate, diltiazem, quinidine, verapmil, Lidocaine. Gitoxin, Digitoxigenin, Quinidine and oxyprenolol.

Unit III: Psychoactive Drugs **(08 Lectures)**

Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs – the neuroleptics, antidepressants, butyrophenones, sernndipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide.

Unit IV: **Anticancer & Antimicrobial Drugs** **(07 Lectures)**

Major scaffolds of anticancer drugs. Quinolone, Mechanism of action, Non-benzoid nitro compounds, nitrofurans, parasitic diseases, Chemotherapy of malaria, 8 & 4-aminoquinolines, other antiprotozoal drugs, antifungal drugs Imidazole compounds, mechanism of action of imidazoles, antihelmintics, antiviral chemotherapy.

Books Recommended:

1. Introduction to Medicinal Chemistry, A. Gringauge, Wiley-VCH.
2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Edited by J.N. Delgado and W. A. Remers, J.B. Lipincott Company.
3. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, AcademicPress.
4. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley & SonsLtd.
5. A Text Book of Medicinal Chemistry, Vol-I and Vol-II, Surendra N. Pandeya, SGPublishers.
6. An Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International Publishers.
7. Medicinal Chemistry, Ashutosh Kar, New Age International Publishers.

CHM20-DSE-303 **Non-equilibrium Thermodynamics & Quantum Chemistry**
Time 30 Hours **Credit: 02**

Unit I: Non Equilibrium Thermodynamics-I (07 Lectures)

Basic principles of non-equilibrium thermodynamics: Second law of thermodynamics for open system, law of conservation of mass, charge and energy. Irreversible processes and uncompensated heat, degree of advancement, reaction rate & affinity, Relation of uncompensated heat to other thermodynamic functions.

Unit II: Non Equilibrium Thermodynamics-II (08 Lectures)

Gibb's equation, entropy production, entropy production due to matter flow, heat flow, chemical reactions, charge flow; entropy production and efficiency of galvanic cells.

Concept of forces & fluxes, Onsager's theory of irreversible processes, phenomenological laws, their domain of validity. Principle of microscopic reversibility and Onsager relations, Chemical reactions near equilibrium. Curie–Prigogine principle. Transformation properties of forces and fluxes.

Unit III: Quantum Chemistry-III (07 Lectures)

Chemical Bonding: Hybridization of orbitals (sp, sp^2&sp^3). Huckel's Pi-MO theory: Application to linear and cyclic polyenes. Pi-electron charge and bond-order. Alternant hydrocarbons, Naphthalene, heteroatomic conjugated systems. Limitations of Huckel theory. Parisar-Parr-Pople method, Extended Huckel Method,

Unit IV: Quantum Chemistry-IV (08 Lectures)

Self-consistent field method: Hamiltonian and wave function for multi-electron systems. Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree and Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H_2 system, Born Oppenheimer approximation; Slater codon rules; Hartree flock equation; Koopman and Brilloiun theories; Roothan equation; Gaussian basis sets

Books Recommended:

1. Thermodynamics of IrreversibleProcesses;DeGroot,Mazur;Dover;1986.
2. Introduction to Thermodynamics of Irreversible Processes; I.Prigogine; Wiley Interscience; 1967.
3. Thermodynamics for students of Chemsitry, Kuriacose, Rajaram, (S. ChandandCo., 1996).
4. Exploring Complexity, I.Prigogine, G. Nicolis, (Freeman, 1998).
5. Molecular Thermodynamics, D. A. McQuarrie, J. D. Simon, USB, 1998.
6. Introduction to Quantum chemistry; A. K. Chandra; Tata McGraw Hill; 1997.
7. Quantum Chemistry - Ira. N. Levine, Prentice Hall, 2000.
8. Quantum Chemistry, Prasad, New Age Publishers, 2000.

CHM20-OGE-301 **Chemistry & Life**
Time: 60 Hours **Credits:04**

Unit 1: Water-An Amazing Chemical Stuff (15 Lectures)
Molecular structure and its unique properties. Composition of natural water. Hard and Soft water. Standards for drinking water. Major causes of water pollution. Contamination of water: Chemical substances affecting potability, color, turbidity, odour, taste, pH and conductivity of water. Methods of treatment of water for domestic and industrial purposes: Sedimentation, Coagulation, Filtration, Sterilization, Break point Chlorination, Flocculation & Fluorination, demineralization and reverse osmosis. Determination of alkalinity of water. Water borne diseases.

Unit II: Fossil Fuels-Coal, Oil & Natural Gas (15 Lectures)
Coal: Formation of Coal deposits. Types & composition of coal. Fuel value of various coals. Analysis of coal: Proximate and ultimate analysis. Significance of fuel gas analysis. Carbonization of coal. Manufacture of metallurgical coke by Otto Hoffman's by product-oven. Oil & Natural Gas: Formation of oil fields, composition & chemical structures of petroleum products. Refining of petroleum, cracking & catalytic reforming. Octane & Cetane rating of fuels. Diesel engine fuel, Kerosene and Gasoline. Lead in petrol: its role, disadvantages & alternatives. LPG & CNG as fuel, addition of mercaptanes to natural gases for safety reasons. Alternative Fuels: Ethanol, Bio-fuels, Bio-gas, Hydrogen & Fuel cells.

Unit III: Polymers & Plastics (15 Lectures)
(a) Characteristics and Types of Polymers. The big six of Polymer**:**Low Density Polyethylene (LDPE), High Density Polyethylene (HDPE), Polypropylene PP), Polystyrene (PS), Polyvinyl Chloride (PVC) and Polyethylene - Tetra phthalate (PET or PETE)- their chemical characteristics and uses. Biodegradable Polymers.

Unit IV: Household Chemicals, Food Additives & Adulterants (15 Lectures)
Chemistry of Soaps, detergents, optical brighteners and bleaching agents, shampoos , conditioners , dyes, hair curling and permanents, deodorants and antiperspirants, perfumes, tooth pastes and sunscreen lotions. **Food Additives:** Flavoring agents, Preservatives (antimicrobial and antioxidant agents). Shelf life of food material. Artificial sweeteners.
Food Adulterants: Adulterants in Milk, Ghee, Oil, Coffee, Tea, Chilli & Turmeric Powders & Pulses. General Food preservatives and their Chemistry, Ripping agents and Pesticides.

Books Recommended:
1. Industrial Chemistry by B.K.Sharma. (Goel publishing House).
2. Applied Chemitry by K.Bagavathi. (Sundan MJP Publishers)
3. Text book of Engineering Chemistry by S.S. Dara. (S.Chand and Co)
4. Engineering Chemistry by M.M.Uppal. & S. Bhatia. (Khanna Publishers)
5. Engineering Chemistry by J.C.Kuricose & J.Rajaram (Tata McGraw Hill)
6. General Organic and Bio-chemistry by Bettelheim and Brown. (Campbell books/cole) – 2009.
7. Principles of Modern Chemistry; 2nd edn; Oxtoby and Nachtrieb; Saunders College Publications; 1987.
8. Chemistry Fundamentals An Environmental Prospective; 2nd edn; Buell and Girad; Jones and Barlett; 2013.

Syllabus for 2 Year M.Sc. Programme in Chemistry (Under CBCS)
(Semester-IV)

Specialization in Inorganic Chemistry

CHM20-CC-401 **Organo-Transition Metal Chemistry**
Time: 60 Hours **Credits: 04**

Unit I: Sigma Bonded Organometallic Compounds (15 Lectures)
Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α-and β hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung. Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

Unit II: Pi-bonded Organometallic Compounds (15 Lectures)
Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.
Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, Structure and bonding of Ferrocene. Compounds with Transition Metal to Carbon multiple bonds: Alkylidene (Schrock and Fischer) Synthesis; Structural characteristics; Nature of bonding. Reactions and their synthetic applications.

Unit III: Catalytic Processes involving Transition Metal Organometallic Compounds (15 Lectures)
Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR). Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis. Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes. Photo redox , Asymmetric and supported Organometallic Catalysis (brief idea)

Unit IV: Fluxional Organometallic Compounds & Synthetic Reactions involving Organometallics (15 Lectures)
Fluxional Organometallic Compounds: Characteristics; Rates of rearrangement and Techniques of study. NMR study of Fluxional behavior, Classification of Fluxional Organometallic Compounds. Mechanism of Fluxionality in compounds of 1 Cyclopentadienyls and 3–allyls. Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation). Synthetic Reactions involving Organo- metallics: Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo's rules). Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes. Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 6th edn; Robert. H . Crabtree; Wiley; 2014.
2. Fundamental Transition Metal Organometallic Chemistry; Charles M. Lukehart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2007

4. Principles and Applications of Organotransition Metal Chemistry; Collman & Finke; University Science Books; 1994.
5. Principles of Organometallic Chemistry; 2nd edn.; P.Powel; Chapman & Hall; 1998.
6. Metallo-Organic Chemistry; A.J.Pearson; Wiley.
7. Mechanisms of Inorganic and Organo metallic reactions; Twigg; Plenum press 1983.
8. Reaction Mechanism of Inorganic and Organometallic systems; 3rd edn.; Robert .B. Jordan, Oxford University Press 2007.
9. Inorganic Chemistry ; 4th edn.; J. Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;2009
10. Modern Inorganic Chemistry; William. A. Jolly; 2nd edn. McGraw Hill; 1991.
11. Principles of Inorganic Chemistry; 1st edn.; Brain W. Pfennig; Wiley; 2015.

CHM20-CC-402 **Photo-Inorganic Chemistry**
Time: 60 Hours **(04 Credits)**

Unit I: Basics of Photo-Chemistry (15 Lectures)

Absorption; mechanism of absorption of light Transition moment integral, Einstein's treatment, molar integrated absorption intensity, natural radiative lifetime & the calculation of life times. Excited states; term symbols, splitting of terms in ligand field, Orgel diagram; electrostaticdescription of spin allowed d-d transitions & energy level diagrams depicting excited states.

Frank Condon principle, shapes of absorption & emission bands. Fate of excited states; energy dissipation by radiative and non-radiative processes. Jablonski diagram.

Tools and Technique: Light source, measurement of light intensity, chemical actinometry. Flash photolysis.

Unit II: Chemistry of Excited State Molecules (15 Lectures)

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non- adiabatic. Properties of thexi states; Determination of dipole moments & acidity constants of excited state molecules.

Photosubstitution reaction of Cr (III) and Rh (III) complexes. Photo reactions of metal carbonyls and metal-metal bond cleavage.

Unit III: Redox Reactions by Excited Metal Complexes (15 Lectures)

Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Marcus-Hush model. Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer, $[Ru (bipy)_3]^{2+}$ and $[Os (bipy)_3]^{2+.}$

Photochemical supramolecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines. Synthetic applications of $[Ru(bipy)_3]^{2+}$ photoredox catalysis (selected examples)

Unit-IV Solar Energy-Prospects & Challenges (15 Lectures)

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO_2 reduction. Inorganic photolithography.

Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

Books Recommended:

1. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
2. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
3. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
4. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
5. Chemistry of Light; Suppan, Royal Society; 1994.
6. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
7. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
8. Inorganic Photochemistry; J.Chem Edu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.

CHM20-CC-403 Advanced Laboratory Course in Inorganic Chemistry
Time: 180 Hours (04 Credits)

A: Multistage Inorganic Preparations and Derivatization: **(04 Experiments)**

i) Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.

ii) Preparation of trans-dicholoro bis-(ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.

iii) Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis-(ethylenediamine) nickel (II) chloride.

iv) Preparation of pentaamminecholorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaammminenitritocobalt (III) chloride and to nitro isomer followed by IR characterization.

B: Analysis of a coordination compound for determination of various components present by bench top methods. **(01- Experiment).**

C: Mixture Separation and Estimations: (02 Experiments)

i)Separation of Permanganate and dichromate ions on alumina column and their estimation from Beer Law plots.

ii) Separation of cobalt (II) and nickel (II) on anion exchange column and their estimation by EDTA titrations.

D. Potentiometric Titrations: (04 Experiments)

i)Determination of transition potential of ferroin redox indicator and purity of Ce (IV) sulphate with a standard iron (II) solution.

ii) Simultaneous determinations of chloride and iodide ions with standard $AgNO_3$.

iii) Establish composition of the complex $K_2Zn_3[Fe(CN)_6]_2$ by using Ferro cyanide with standard Zinc (II) complexometric titration.

iv) Complexation effect on redox potential of iron redox couple: Simultaneous potentiometric estimation of iron binary and ternary complex mixtures.

E. pH-metric Titrations: (02 Experiments)

• Quantitative analysis of Chromate Dichromate mixture by pH Titration.

• pH influence on the pH dependent iron(II) dichromate redox reaction monitored by potentiometry.

F. Conductometric Titrations: (02 Experiments)

• To determine solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.

• Conductometric investigation of silver(I) ethylenediamine complexation reaction.

G. Spectrophotometry: (03 Experiments)

• Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation.
• Determination of composition of Iron (II)-2,2-bipyridyl complex by Mole ratio method.
• Determination of rate of aquation of complex [Co $(NH_3)_5Cl]$ Cl_2 in acidic medium.

H. Advanced/demonstrative type experiments: (non-evaluative)

i) BSA/ DNA binding ability of metal complex using absorption and emission techniques.
ii)Cyclic Voltammetric behavior of trisphenanthroline iron(II) complex.
iii) Synthesis, morphological analysis and particle size determination of metal nanoparticles.
iv) Photocatalytic degradation of the commercial dye using some nanomaterials.

Books Recommended:

1. Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education2002
2. Synthesis and Technique in Inorganic chemistry, G. S.Girlomi; R.J. Angleci 3rdEdn.; University Science Books.
3. Synthesis and characterization of Inorganic compounds W.AJolly
4. Inorganic syntheses Vols II, VI AcademicPress.
5. Experimental Inorganic / Physical Chemistry ; Mounir A. MalatiHorwood/1999.
6. Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
7. Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ;1995
8. Journal of Chemical Education vol. 88(2), year 2011,pp.220-222.
9. Russian Journal of general Chemistry, vol 85, year 2015, pp.959-973.
10. Journal of Chemical Education vol. 93(2), year 2016,pp.355-361.
11. Journal of Chemical Education vol. 68(8), year 1991,pp.677-678.
12. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH,2003)
13. Experimental Electrochemistry---R. Holze (Wiley-VCH,2009).

CHM20-DSE-401 **Biological Inorganic Chemistry**
Time: 30 Hours **Credits: 02**

Unit I: Metallo-enzymes & Electron Carriers **(08 Lectures)** Zinc enzymes: Carboxypeptadiase and Carbonic Anhydrase: Introduction, Structure, Mechanism of action and their model compounds.
Biological chemistry of Molybdenum: uptake of Molybdenum; oxidation states and redox Potentials in enzymes and oxygen atom transfer reactions.
Cobalt in Vitamin B12: Introduction, Structure and Derivatives of B12 and mechanism of alkylation reaction.
Electron Carriers: Rubredoxin & Ferridoxin (Structure and biological role).
Blue Copper proteins: Oxidases and Plastocyanin (Structure and biological role).

Unit II: Metal-ion Induced Toxicity and Chelation Therapy **(08 Lectures)**
Mechanism of metal ion induced toxicity: Toxicity of Pb, Cd, Hg, As, and CN.
Metal ion promoted Carcinogenesis and probable mechanism of action.
Therapeutic Aspects of Chelating Drugs: Conditional stability constant, Stereochemistry, Lipophilicity. HSAB and Plasma mobilizing index(PMI).
Types of Chelation Therapy: Single, Double, Synergistic and Mixed ligand chelation therapy. Therapeutic index of different chelating drugs in metal ion detoxification.
Radio protective chelating drugs. Limitations and Hazards of Chelation therapy.

Unit III: Metal Complexes in Therapeutics **(07 Lectures)**
Treatment of essential metal deficiencies. Metal salts as anti-acids, antiseptic and diuretics.

Gold compounds and Rhematoid arthiritis. Anti-Cancer Drugs: cis-Platin and its derivatives. Structure-function relationship. Anti-bacterial, Anti-viral and Anti-fungal activities of Metal Complexes with probable mechanism of action. Metal complexes in radio-diagnosis Photodynamic therapy: concept and applications.

Unit IV: Metal Complexes as ligands to Biotargets (07 Lectures)

Absorption, fluorescence, Circular Dichromism spectroscopies in investigating interaction of metal complexes with biological targets (DNA, BSA and enzymes). Cytotoxicity evaluation assays and Gel Electrophoresis. Deciphering binding modes, thermodynamics and mechanism of drug interaction using selected metal complex case studies.

Books Recommended:

1. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
2. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.
3. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
4. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley; 1973.
5. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
6. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
7. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.

CHM20-DSE-402 Non-Aqueous, Supramolecular & Inorganic Polymer Chemistry
Time: 30 Hours Credits: 02

Unit I: Reaction in Non-aqueous Solvents (08 Lectures)

Classification of Non-aqueous solvents; Comparison of aqueous and non-aqueous solvents, details of important chemical reactions in liquid H_2SO_4, NH_3, SO_2, BrF_3 and N_2O_4.

Unit II: Supramolecular Chemistry-I (08 Lectures)

Host-guest interactions, intermolecular forces, nature of supramolecular interactions.
HSAB Concept-: classification, symbiosis. Utility in drug design, molecular recognition.
Soft Ligands for soft metal ions-mixed crown ethers and mixed Cryptands.
Cation binding hosts: Supramolecular cation coordination chemistry, introductory account of cation receptors: Podands, corands, cryptands, spherands, siderophores and calixarenes.

Unit III: Supramolecular Chemistry-II (07 Lectures)

Hosts to Anion: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series,
Introductory account of anion receptors - cyclophanes, pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns, neutral receptors.
Hosts for Neutral receptors: clathrates, inclusion compounds, zeolites.
Ion Pair Receptors: contact ion pairs, cascade complexes.

Unit IV: Inorganic Polymers (07 Lectures)

Classification, Inorganic Polymeric Reactions: Condensation, Addition, and Coordination. Significance of Coordination polymers. Preparations, properties, structure-bonding and applications of polymeric sulfur, sulfur nitrides, polyphosphates and Silicones:

Books Recommended:

1. The Chemistry of Non aqueous solvents; Vols II & III Lagowski; Academic Press.

2. Advanced Inorganic Chemistry, 5th edn; F.A.Cotton & G.Wilikinson; Wiley;1988.
3. Supramolecular Chemistry. Jonathan W. Steed and Jerry L. Atwood. Wiley 2nd Edn.
4. Supramolecular Chemistry - Fundamentals and Applications. A. Katsuhiko and K. Toyoki. Springer.
5.An Introduction to Supramolecular Chemistry. Asim K. Das, Mahua Das, CBS Publishers and Distributors Pvt Ltd. 2005
6. Supramolecular Chemistry J. M. Lehn, Wiley-VCH
7. Principles and Methods in Supramolecular Chemistry; H-J Schneider, A Yatsimirsky; John Wiley,2000.
8.. Inorganic Polymers NJ Ray; Academic Press; 1978.
9. Inorganic Polymers James. E.Mark, HarryAllock & Roberta West; Prentice Hall.
10. Inorganic Polymers F.G-A-Stone & W. A. Graham; Academic Press.

Specialization in Organic Chemistry

CHM20-CC-404 **Chemistry of Natural Products**
Time: 60 Hours **Credits: 04**

Unit I: Terpenoids & Carotenoids (15 Lectures)
Introduction, Isoprene rule, classification, occurrence, general method of isolation, separation and structure elucidation of terpenoids. Structure determination, stereochemistry and synthesis of plant Citral, α-terpeneol, juvenile hormone, Zingiberene, α-santonin and Phytol. Structure determination and synthesis of β-carotene. Biogenesis of terpenoids. Upto sesqi- terpenoids.

Unit II: Alkaloids & Marcolactones (15 Lectures)
Definition, classification, nomenclature and physiological properties of alkaloids. Occurrence, qualitative tests, isolation and general methods of structure elucidation. Role of alkaloids in plants**.**
Chemistry of important alkaloids: Ephedrine, Quinine, Nicotine and Morphine. Biogenesis of alkaloids.
Chemistry of important Marcolactones (erythromycin and amphotericin B). Biogenesis of alkaloids.

Unit III: Steroids (15 Lectures)
Introduction, nomenclature, classification & stereochemistry. Qualitative tests.
Cholesterol: Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.
Sex hormones: Introduction, isolation, clinical & commercial significance. Color reactions. Structure determination and partial synthesis of Aldosterone, Testosterone and Progesterone.
Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis. Mechanism of action and synthesis of cholecalciferol.

Unit IV: Prostaglandins & Flavonoids (15 Lectures)
Flavonoids: Introduction, classification, occurrence, qualitative tests and general chemical and spectral methods of structure determination of flavonoids.
Structure determination and synthesis of chrysin, quercetin, genestin and cyanidine.
Porphyrins: Structure features of heme and chlorophyll.
Prostaglandins: **I**ntroduction, structural features, physiological functions and medicinal uses of Prostaglandins. Synthesis/biosynthesis of PGE_2 and PGF_2-α.

Books Recommended:

1. Chemistry of Natural Products; S. V. Bhat, B. A. Nagasampagin. (Narosa 2005).
2. Organic Chemistry, 5th Ed. Vol.1.L. Finar (Addison Wisley Longman-2000).
3. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

CHM20-CC-405 **Reagents & Designing Organic Synthesis**
Time: 60 Hours **Credits: 04**

Unit I: Application of reagents in Organic Synthesis (15 Lectures)

Oxidation: Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using Jone's reagent, PCC, Swern reagent and Dess-Martin Periodinane (DMP). Oppeneauer oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide and Manganese(III)acetate. Fetizon oxidation. Prevost hydroxylation and its modification by Woodward.

Reduction: Introduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using $LiAlH_4$, $NaBH_4$ and Red-Al, Bouveault-Blanc reduction, Corey-Bakshi-Shibata (CBS) reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride and Lithium triethylborohydride (superhydride).

Unit II: Protection & Interconversion of Functional Groups (15 Lectures)

Protection of functional groups: Principle of protection of functional groups and its significance. Protection of carbon-hydrogen bonds (in terminal alkynes and Carbon-hydrogen bond of aldehydes), carbon-carbon double bonds, alcoholic and Phenolic hydroxyl groups, amino groups, carbonyl and carboxyl groups. Functional Group Interconversion (FGI) / Transformations: Significance of Functional Group Interconversion (FGI) / Transformations in Organic synthesis. Methods of transformation of different functional groups into one another. Chemoselectivity.

Unit III: Designing Organic Synthesis-I (15 Lectures)

The disconnection approach: Introduction to synthons, their types and equivalent reagents. Reversal of Polarity (umpolung). One group, two group and Reteroelectrocyclic disconnections. Reterosynthetic Analysis involving connections and rearrangements. Guidelines for good disconnections. Reterosynthetic analysis of alcohols, amines (aliphatic and aromatic), alkenes, carbonyl compounds, carboxylic acids and their derivatives using one group disconnections and FGIs. Use of acetylenes in the syntheses of above mentioned compounds.

Unit IV: Designing Organic Synthesis-II (15 Lectures)

Two group disconnections: Reterosynthetic analysis of 1, 2- difunctional compounds (1,2 – diols), 1,3- difunctional compounds (1,3-dioxygenated compounds, α, β - unsaturated carbonyl compounds, 3-amino alcohols and 3- amino ketones), 1,4- and 1,5- difunctional compounds.Multistep Synthesis: Application of retrosynthetic analysis in designing /achieving syntheses of some complex molecules (for example Brufen, benziodarone, Juvabione, warfarin and brevicomin).

Books Recommended:

1. Designing Organic Synthesis, S. Warren ;Wiley; 2013.
2. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 2007.
5. Organic Chemistry, 10th edn;. T. W. G. Solomons and Craig B. Fryhle ; Wiley-2012.
6. Organic Chemistry; Clayden, Greeves, Warren and Wothers ; Oxford University Press-2012.
7. Organic Chemistry, David Klein; John-Wiley-2012.
8. Advanced Organic Chemistry: Reactions, Mechanism and Structure, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013.

CHM20-CC-406 Advanced Laboratory Course in Organic Chemistry
Time: 180 Hours Credits: 04

1. Use of chemistry software like Chem draw, Chem office etc.
2. (a) Isolation of caffeine from tealeaves
(b) Isolation of piperine from black pepper
(c)Isolation of lycopene fromtomatoes.
3. Preparations, isolation and characterizations: (one/two/three-stage).
3.1 3.3 Synthesis of indole from cylohexanone andphenylhydrazine.
3.4 Para- aminoazobenzene fromaniline
3.3.7 Benzoin → Benzil → BenzilicAcid.
3.8 Nitrobenzene →m-dinitrobenzene → m-nitroaniline →m-nitrophenol.
3.9 Pthalic anhydride → phthalimide → anthranilicacid.
3.10 Eosin from phthalicanhydride
3.11 Glucazone fromglucose
3.12 Methylene blue from dimethylaniline.

Books Recommended:

1. Vogel Practical OrganicChemistry.
2. Comprehensive Practical Organic Chemistry by V.K.Ahluwalia.
3. Advanced practical (organic chemistry) by N. K.Vishnoi.

CHM20-DSE-403 Basic Organic Reactions-The Biological Connection
Time: 30 Hours Credits: 02

Unit I: Substitutions Reactions (07 Lectures)

Nucleophilic substitutions: Chemical and enzymatic hydrolyses of glycosidic bonds-An example of SN reaction. Mustard gas and treatment of neoplastic disease. Benzo [a] pyrene

and nitrosoamines and cancer. Biological S_N1 reaction involving allyl cations. Biosynthesis of glycosides via UDP sugars-A S_N2 process. N-Acetylation of amino sugars.
Esterificaiton in oils and fats. Transesterification: Prohibition of biosynthesis of prostaglandins by Aspirin. Transesterification of triglycerides with ethanol to get biodiesel. Examples of substitution reactions in biological systems.

Unit II: Addition Reactions (07 Lectures)
Electrophilic additions: Electrophilic addition to carbocations in Terpenes. Alkylation of steroidal side chain during biosynthesis of Lanosterol to Ergosterol, Stigmasterol and β-Sitosterol. Nucleophilic addition to carbonyl group. Amide formation during synthesis of peptides and proteins. Unique structure of amide bond.
Addition of alcohols to carbonyl group: Hemiacetal and Acetal formation in sugars. Formation of glycoside: Chemistry and Stereochemistry.
Enzyme catalysed addition to α, β-unsaturated carbonyl compound. Michael acceptors as Carcinogens.

Unit III: Condensation Reactions (08 Lectures)
Aldol reaction between formaldehyde and glycoaldehyde and formation of glycoaldehyde through benzoin condensation between formaldehyde and HCN during biosynthesis of carbohydrates.
Claisen and Aldol reactions in nature.
(a) HMG-CoA and Mevalonic acid.
(b) In biosynthesis of phenols.
(c) Claisen reaction involving Acetyl Coenzyme A and Malonyl Coenzyme A
(d) Reverse Claisen reaction: β-oxidation of fatty acids.
(e) Nature's enolates: The lysine enamines and coenzyme A.

Unit IV: Biological Oxidation–Reductions (08 Lectures)
Oxidations in biological systems: Autoxidation in fats and oils–The origin of rancidity. Natural antioxidants Antioxidants-mechanism of action Radical oxidation in prostaglandins. Oxidative phenol coupling in biosynthesis of morphine /thyroxine. Biological oxidation of pregnelonone to progesterone and cholesterol to choles-4-ene-2-one. Mechanism of oxidations by FMN and FAD. Oxidation of alcohols by NAD+.
Reduction in biological systems: NADH and NADPH-The biological equivalents of NaBH4. Reductions by FADH2 and FMNH2. Reductive amination in nature.

Books Recommended:

1. Advanced Organic Chemistry; 5th edn; F. A. Carey and R. J. Sundberg; Plenum; 2007.
2. Reaction Mechanism in Organic Chemistry; 3rd edn; S.M. Mukherjee and S.P. Singh; Macmillan; 1998.
3. Fundamentals of Organic Chemistry; 10th edn; Solomons; Wiley; 2012.
4. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2012).
5. Advanced Organic Chemistry 4th Ed. - F. A. Carey and R. J. Sundberg. (Plenum, 2001).
6. Chemistry of Natural Products; S. V. Bhat, B. A. Nagasampagin. (Narosa 2005).
7. Organic Chemistry, 5th Ed. Vol.1.L. Finar (Addison Wisley Longman-2000).
8. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
9. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
10. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006

CHM20-DSE-404 **Heterocyclic Chemistry**
Time: 30 Hours **Credits: 02**

Unit I: Introduction of Heterocyclic Compounds (07 Lectures)
Introduction, significance and structural features and nomenclature of different types of heterocyclic compounds.
Spectral properties of heterocycles. Tautomerism in heterocycles.

Unit II: General Approach to Synthesis of Heterocyclic compounds (07 Lectures)
Reactions most frequently used in heterocyclic ring synthesis like C-C bonding, C-heteroatom bonding, typical reactant combinations , Electrocyclic processes in heterocyclic ring synthesis, Nitrenes in heterocyclic synthesis, Hantzsch Pyridine, Skraup quinoline, Bischler-Napieralki Isoquinoline, Knorr Pyrrole, Paal-Knorr, Fischer-Indole synthesis.

Unit III: Monocyclic Heterocycles (08 Lectures)
Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines, Pyridine. Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles. Chemistry of Six membered rings like Azines and seven membered heterocycles like Azepine, Oxipene, Thiepins. Utility of these compounds in day today life.

Unit IV: Bicyclic Heterocycles (08 Lectures)
Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan, Benzo-thiophene, benzotriazole, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2- and 4-benzopyrones, Benzopyryllium salts and purines. Applications in chemistry and biology.

Books Recommended:
1. Heterocyclic Chemistry, 5th Ed. J. A. Joule and K. Mills, (Wiley-2010).
2. Essentials of Organic Chemistry, Paul M Dewick, (Wiley-2006).
3. Heterocyclic Chemistry, J.A. Joule and G. F. Smith, (Chapman and Hall-1996).
4. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann, (George Thieme Verlag Stuttgart, New York -1995).
5. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
6. Heterocyclic Chemistry, R. R. Gupta, M. Kumar, V. Gupta, (Springer-2006).

Specialization in Physical Chemistry

CHM20-CC-407 **Advanced Quantum Chemistry**
Time: 60 Hours **Credits: 04**

Unit I: Electronic Structure Theory, Hartree-Fock Method (15 Lectures)
Review of Electronic Hamiltonian, anti-symmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H2 system.

Hartree-Fock Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure.
Basis Sets: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on Helium, H_2 /HeH+.

Unit II: Configuration Interaction & Semiempirical Methods (15 Lectures)
Configuration Interaction: Electron correlation, configuration state functions, configuration interaction (CI), Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.
Semiempirical methods: The ZDO approximation; brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit III: Density Functional & Semi-Empirical Methods (15 Lectures)
Density Functional Theory: Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, Ex & Ec functionals; the local density and local spin density approximations, gradient corrected functional.
Brief idea of Molecular mechanics methods, force fields.
Molecular Properties: Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit IV: Use of Quantum Chemistry Software: Gaussian (15 Lectures)
A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package..
1. A single point energy calculation: HCHO /CH3.CO.CH3, HCHO MOs
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization $–C_3H_5F$
7. Model Chemistries: Basis set effect on HF bond length
8. Selecting an appropriate theoretical method:
a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
b) Density Functional Theory: CO_2 structure and atomization energy.
c) Butane/Isobutane isomerization energy, rotational barrier in n-butane.
9. Chemical reactions and reactivity:
(a) Electron densities of substituted benzenes.
(b) Hydration enthalpy of the reaction $H+ + H_2O \rightarrow H_3O+$
(c) Potential energy surfaces. Reaction path following (IRC calculation) CH2O → HCOH
(d) Heat of formation of CO2 via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile.

Books Recommended:
1. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry, 2nd Edn , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)

5. Molecular Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
7. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
8. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
9. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

CHM20-CC-408 Statistical Mechanics & Advanced Electrochemistry
Time: 60 Hours Credits: 04

Unit I: Classical Statistical Mechanics & Ensemble concept (15 Lectures)

Equations of Motion; Newton, Lagrange and Hamiltonian. Classical partition function, phase space and the Liouville equation, Kinetic theory of gases, equi-partition of energy, Maxwell's velocity distribution

Concept of ensembles, ensemble average and postulate of equal a priori probability. Canonical, grand-canonical and Micro-canonical ensembles. Ensemble partition functions and related thermodynamic functions. Ideal gas in canonical and Grand canonical ensemble.

Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand partition function, virial coefficient in the classical limit, second and third virial coefficients.

Statistical thermodynamics of solutions: Lattice model, regular solution theory, Statistical Mechanics of polymer solution.

Unit II: Quantum Statistics (15 Lectures)

Quantum Statistics: Fermi-Dirac and Boson-Einstein statistics, Nuclear spin statistics, symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO. Application of grand partition function to Boson-Einstein and Fermi-Dirac statistics. Ideal Fermi-Dirac gas: Electrons in metals, Ideal Photon gas: Black body radiation.

Heat capacity of solids, Einstein and Debye models (Partition function, Average energy and heat capacity). Limitations of the models.

Unit III: Instrumental Methods in Electrochemistry (15 Lectures)

Fundamentals: Electrode potential and its measurement, Standard and formal electrode potentials, three electrode measurements, uncompensated resistance. Overview of Electrode Processes-Faradaic and Non-Faradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1st and 2nd law of diffusion, Cottrell equation.

Electrochemical Techniques: Potential Step Methods: Chronoamperometry, Chronocoulometry at macroelectrodes; theory and applications.

Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macroelectrodes theory and applications, Diagnostic criteria of Cyclic Voltammetry.

Unit IV: Applied Electrochemistry (15 Lectures)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications, mechanism and approach to bioelectrosynthesis, examples of bioelectrosysnthesis- oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Energy storage devices: Desirable characteristics of energy storage devices, Batteries, Classical Batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide), Modern Batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries), Supercapacitors.
Fuel cells, Types of Fuel Cells (Alkaline, Phosphoric acid, Polymer Electrolyte membrane and Direct MeOH fuel cell), Biofuel cells.

Books Recommended:

1. Electrochemical Methods Fundamentals and Applications, 2nd Edition, Allen J. Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
3. Understanding Voltammetry, 2nd Edition, Imperial College Press.
4. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
5. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.
6. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
7. Statistical Thermodynamics, M. C. Gupta, (New Age International, 1993).
8. Statistical Thermodynamics-Fundamentals and Applications, N. M. Laurendeau, Cambridge University Press, 2005.
9. Statistical Mechanics, D. A. McQuarrie, (Viva, 2003).
10. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
11. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover, 1990).
12. Statistical Mechanics - Principles and Applications, Hill, Dover, 1987.
13. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
14. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley, 1987).

CHM20-CC-409 Advanced Laboratory Course in Physical Chemistry
Time: 180 Hours Credits: 04

A. Tensiometry

1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

B. Cryoscopy

1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

C. Spectrophotometry

1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.
3. Isolation and spectrophotometric characterization of nucleic acids from Onion or Peas or Liver.

D. Spectrofluorometry

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl4 in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

E. Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

F. Dynamic Electrochemistry

1. Estimate the surface area of a working electrode through Chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry determine the formal potential and diffusion coefficient of $[Fe(CN)_6]3-$.
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

G. Kinetics

1. Kinetic Investigation of BZ-Oscillatory reaction.
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

I. Viscometry and densitometery

1. Determination of Mol. Mass of a Polymer (Polyvinyl alcohol) using viscosity method.
2. Explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended:

1. Practical Physical Chemistry --- Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry---R. Holze (Wiley-VCH, 2009).

CHM20-DSE-405 **Chemistry of Materials**
Time: 30 Hours **Credits:2**

Unit I: Langmuir Blodgett Films & Liquid Crystals (08 Lectures)

Langmuir- Blodgett Films: Introduction and general preparative techniques. LB Films of various compounds (hydrocarbon, liquid crystals compounds and polymers), Applications – nonlinear optical effects, conduction, photoconductivity and sensors.
Liquid Crystals: Mesomorphism, types of liquid crystals, molecular structural requirement of mesomorphism, properties of liquid crystals, Applications – Liquid crystal displays, thermography, optical imaging and ferroelectric liquid crystals.

Unit II: Organic Solids & Molecular Devices (07 Lectures)

Organic solids and fullerenes: Organics conductors, magnetism in organic materials. Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes)
Molecular devices: Molecular rectifiers and transistors, artificial photosynthetic devices, switches and sensors.

Unit III: Optical Materials (07 Lectures)
Luminescence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducting lasers, quantum cascade and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Unit IV: Solid electrolytes & High Tc Superconductors (08 Lectures)
Ionic Conductors: Introduction to ionic conduction, types of ionic conductors, mechanism of ionic conduction- interstitial jumps (Frenkel) and vacancy mechanism. Super-ionic conductors: Diffusion and transition superionic conductors. Examples and applications of ionic conductors.
High Tc superconductors: Superconductors: Properties and types. high Tc superconductivity in cuprates: Structure and preparation of 1-2-3 materials, mechanism of high Tc superconductivity, Applications of High Tc materials.

Books Recommended:

1. Solid State Chemistry and its Applications, West, Wiley, 2014.
2. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
3. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders College, 2001.
4. Principles of Solid State, H. V. Keer, Wiley Eastern; 2008.
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
7. New directions in solid state chemistry, C.N.R. Rao and J. Gopalakrishnan, Cambridge University Press, 2nd ed. 1997.
8. Introduction to superconductivity, Micheal Tinkham, Dover books, 2nd ed. 2004.

CHM20-DSE-406 Advanced Photochemistry & Radiation Chemistry
Time: 30 Hours Credits: 02

Unit I: Photochemistry-I (07 Lectures)
Molecular photochemistry: Transitions between states (Chemical, classical and quantum dynamics, vibronic states). Potential energy surfaces; transitions between potential energy surfaces, The Franck-Condon Principle and radiative transitions. A classical model of radiative transitions. The absorption and emission of light - state mixing, spin-orbit coupling and spin forbidden radiative transitions, absorption complexes, delayed fluorescence and phosphorescence.

Unit II: Photochemistry-II (08 Lectures)

Photophysical radiationless transitions*:* Wave mechanical interpretation of radiation less transitionsbetween state factors that influence the rate of vibrational relaxation. Energy transfer: Theory ofradiationless energy transfer, energy transfer by electron exchange: An overlap or collisionmechanism. The role of energetics in energy transfer mechanism. Diffusion controlled quenching. ThePerrin formulation. Triplet-triplet, triplet-singlet, singlet-triplet energy transfer. Multiphoton energytransfer processes, reversible energy transfer.

Unit III: Radiation Chemistry & Dosimetry (08 Lectures)

An overview: G-value. The mechanism of interaction of high energy radiation with matter, Photoelectric effect, Compton effect, Pair production, total absorption co-efficient, excitation and ionization, Stopping power and linear energy transfer.

Radiation dosimetry: Radiation dose and its measurement, standard free air chamber method, chemical dosimeter (Frick's Dosimeter). Short lived intermediates (ions, excited molecules, free radicals: Various mechanisms of their formation and energy transfer processes).

Unit IV: Photolysis (07 Lectures)

Flash photolysis: Principle and its applications. Radiolysis of water and aqueous solutions. Radiolysis of molecules of biological interest (carbohydrates, amino acids, peptides, and nucleic acids).

Books Recommended:

1. Turro, N. J. *Modern Molecular Photochemistry* Univ. Science Books (1991).
2. Gilbert, A. & Baggot, J. *Essentials of Molecular Photochemistry* Blackwell Scientific (1990)
3. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
4. McQuarie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. ScienceBooks (2001).

CHM20-CC-410 **Biochemistry & Chemical Biology**

Time: 60 Hours **Credits: 04**

Unit I: Bio-Physical Chemistry (15 Lectures)

Relevance of thermodynamics to biological systems; standard state, standard energy changes in biochemical reactions. Concept of enthalpy, entropy and free energy changes in cellular reactions. ATP as energy currency of cell in the synthesis & degradation reactions. Principles of coupled reactions and their importance in living systems.

Acid–base Equilibria: pH, pKa & pKb values. Dissociation of Amino-acids, isoelectric point. Buffer solutions with effect of ionic strength & temperature, buffer capacity, maintaining pH of blood. Biological Membranes, Transport of ions across biological membranes, active and passive transport. Theory of membrane potential, Nernst, Plank, Goldman equation in physiological functions & diseases.

Electrochemical equilibria: Standard redox potential, half-cell potentials of biological reaction. Denaturation of DNA & Renaturation of DNA as a second order reaction. Enzyme kinetics, effect of substrate, temperature and pH on reaction rate in biochemical reactions. Michaelis-Menton mechanism; Specificity of enzyme action: types of specificity & the active sites. Enzyme Inhibition: Introduction, Competitive inhibition, Un-Competitive inhibition, Non-competitive, Allosteric inhibition. Multi-substrate systems.

Unit II: Bio-Inorganic Chemistry (15 Lectures)

Macro, Micro, Trace and Ultra-Trace Elements in Biological Systems. Transport mechanism: uniport, symport and antiport of important ions. Ferritin and Transferrin: Structure, metal binding sites; incorporation and release of iron. Porphyrins in biology: Introduction, characteristics of absorption spectrum. Haemoglobin and Myoglobin, mechanism of oxygen transport and storage. Bohr effect and cooperativity in haemoglobin. Chlorophyll: Structure, oxygen saturation curves. Synthetic oxygen carrier model compounds.

Metal ions, cofactors and enzyme action:Carboxy peptidases and Carbonic Anhydrase, Xanthine oxidase and Aldehyde oxidase: Structure and biological role. Cobalt in Vitamin B12: Introduction, structure and derivatives of B12 and mechanism of alkylation reaction. Electron Carriers: Rubredoxin & Ferridoxin. Blue Copper proteins: Oxidases and Plastocyanin in chemico-biological interactions.

Unit III: Bio-Organic Chemistry (15 Lectures)

Significance of bonding (Ionic, covalent and hydrogen) in biochemical reactions with examples from nucleic acids, proteins, carbohydrates & lipids. Significance of H-bonding and Vander waal's interactions for base pairing in nucleic acids.

Sterospecificity in biological reactions with examples from amino-acids and carbohydrates in bacteria, plants and animals. Carbohydrates from Aldol reaction for disaccharides and polysaccharides. Various mechanistic chemical pathways in biological processes including free radical reactions and other reaction types. Proximity effects in bio-organic reactions and molecular rearrangements in metabolic reactions. Significance of methylation and acetylation and various group additions as post-translational modifications in various processes.

Formation of amino acids under prebiotic conditions. Formation of Purines and Pyrimidine's under prebiotic conditions. Reduction in biological systems: NADH and NADPH. Chemical biology approach for pathway elucidations and metabolic regulations.

Unit IV: Bio-Analytical & Bio-Industrial Chemistry (15 Lectures)

Biochemical parameters and analysis. Bio-analysis of physiological components like amino acids, proteins, sugars, fatty acids, hormones etc by chemical methods for diagnosis, prognosis & therapeutics. Quantification of enzymes and their substrates. Immobilized enzymes & Biosensors in human physiology. Use of electrophoresis, centrifugation and mass spectrometry for the analysis of biomolecules. Automatic analyzers for various estimations of biological importance. Bio-Industrial Chemistry: concept, methods & applications. Common processes for important bioactive isolation, purification, characterization & upscaling.

Books Recommended:

1. Foundation of Inorganic, Organic and Biological Chemistry; Cavet, Denniston and Topping; W.C Brown Publication; 1995.
2. Organic and Biological Chemistry; John R. Holum; Wiley; 2001.
3. Essential of Organic Chemistry; Paul M. Dewick; Wiley; 2006.

4. Paula Bruice; Organic Chemistry; Paula Y. Bruice; Pearson; 2012.
5. Organic Chemistry; F.A Carey and Robert Giuliano; Tata McGraw Hill; 8th Ed. 2012.
6. Organic Chemistry; Clayden, Greeves, Warren and Wolthers, Oxford University Press; 2012.
7. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
9. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
10. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005
11. Physical Chemistry for life sciences; 2nd edn.; P. W. Atkins and J.D. Paula; Oxford University Press; 2010.
12. Fundamentals of general Biological Chemistry; 4th edn.; John . R. Holum; Wiley; 1990.
13. Principles of biochemistry; 3rd edn; David. L .Nelson, Michael .M.Cox; Worth Pub.; 2002.
14. Physical Chemistry, Principles and applications in biological systems. 4thedn. Tinoco, Sauer, Wang, Puglisi. Pearson education, 2007.

CHM20-CC-411 **Journal Club & Seminar**
Time: 30 Hours **(Credits: 02)**

*#@Journal Club & **$@Seminar

*Journal Club & **Seminar.

#Each student under the supervision of a Faculty/Advisor will present one original manuscript from a reputed Journal to the Department.

$Each student under the supervision of a Faculty/Advisor will present one Recent Review article(s) based seminar to the Department.

@Departmental Evaluation by Faculty, HOD & Dean, School of Physical & Chemical Sciences.

CHM20-CC-412 **Professional Development & Career Progression**
Time: 60 Hours **(Credits: 04)**

$@**Professional Development & Career Progression**

@Departmental Evaluation by Faculty, HOD & Dean, School of Physical & Chemical Sciences.