

# **MASTER OF SCIENCE IN CHEMISTRY**

## **SYLLABUS FOR THE CREDIT BASED CURRICULUM Two-Years Four Semesters Course**

**From 2019 Onwards**

---



**Department of Chemistry  
Indian Institute of Engineering Science and Technology, Shibpur  
Howrah – 711 103**

**Proposed Course Structure for Two-Year M. Sc Program  
(From 2019 Onward)**

*First Semester*

Sl. No.	Subject Code	Subject Name	Class Load/Week			Total load/Week	Credit	Marks
			L	T	P			
1	CH5101	Paper-I (Core) Quantum mechanics and molecular spectroscopy	3	1	0	4	4	100
2	CH5102	Paper-II (Core) Transition metal chemistry: Structure-bonding correlation, Magnetic properties and Bioinorganic Chemistry	3	1	0	4	4	100
3	CH5103	Paper-III (Core) Stereochemistry, Reaction Mechanism and Heterocyclic Chemistry	3	1	0	4	4	100
4	CH5121/ CH5122	Paper-IV (Departmental Elective): Group Theory and Application of Spectroscopy / Instrumental Techniques for Chemical Analysis	3	0	0	3	3	100
5	CH5161	Paper-V (Open Elective) Chemistry of nanomaterial	3	0	0	3	3	100
6	CH5171	Inorganic Chemistry Laboratory-I	0	0	4	4	2	50
7	CH5172	Organic Chemistry Laboratory-I	0	0	4	4	2	50
<b>Total</b>			<b>15</b>	<b>3</b>	<b>08</b>	<b>26</b>	<b>22</b>	<b>600</b>

Second Semester

Sl. No.	Subject Code	Subject Name	Class Load/Week			Total load/Week	Credit	Marks
			L	T	P			
1	CH5201	Paper-VI (Core) Classical and statistical thermodynamics, surface and bio-physical chemistry	3	1	0	4	4	100
2	CH5202	Paper-VII (Core) Organometallic, Homogeneous catalysis and Solid state chemistry	3	1	0	4	4	100
3	CH5203	Paper-VIII (Core) Synthetic Organic Chemistry	3	1	0	4	4	100
4	CH5221/ CH5222/ CH5223	Paper-IX (Departmental Elective): Green Chemistry, Pericyclic Reactions and Organic Photochemistry / Photophysical processes and polymer chemistry / Advanced bioinorganic and inorganic supramolecular chemistry	3	0	0	3	3	100
5	CH5261	Paper-X (Open Elective): Spectroscopy for Chemical Analysis	3	0	0	3	3	100
6	CH5271	Physical Chemistry Laboratory-I	0	0	4	4	2	50
7	CH5272	Organic Chemistry Laboratory-II	0	0	4	4	2	50
8	CH5273	Term Paper	0	0	8	8	4	100
9	CH5291	Term Paper Viva	0	0	0	0	2	100
<b>Total</b>			<b>15</b>	<b>3</b>	<b>16</b>	<b>34</b>	<b>28</b>	<b>800</b>

Third Semester

Sl. No.	Subject Code	Subject Name	Class Load/Week			Total load/Week	Credit	Marks
			L	T	P			
1	CH6101	Paper-XI (Core) Kinetics, Microscopic Dynamics and Fundamentals of Electrochemistry	3	1	0	4	4	100
2	CH6102	Paper-XII (Core) Reaction Mechanism and Spectroscopic techniques in Inorganic Chemistry	3	1	0	4	4	100
3	CH6103	Paper-XIII (Core) Chemistry of Natural Product and Supramolecular Chemistry	3	1	0	4	4	100
4	CH6171	Inorganic Chemistry Laboratory-II	0	0	4	4	2	50
5	CH6172	Physical Chemistry Laboratory-II	0	0	4	4	2	50
6	CH6173	M. Sc. Thesis Part-I (Progress Report)	0	0	14	14	5	100
	CH6191	Thesis Progress report Seminar and Viva	0	0	0	0	2	100
<b>Total</b>			<b>9</b>	<b>3</b>	<b>22</b>	<b>34</b>	<b>23</b>	<b>600</b>

Fourth Semester

Sl. No.	Subject Code	Subject Name	Class Load/Week			Total load/Week	Credit	Marks
			L	T	P			
1**	CH6201/ CH6202/ CH6203	Paper-XIV (Core) Molecular Quantum Mechanics and Statistical Mechanics / Chemistry of f- block, Photochemistry, Clusters and Crystallography / Advanced Methods in Organic Synthesis	3	1	0	4	4	100
2**	CH6221/ CH6222/ CH6223/ CH6224	Paper-XV (Departmental Elective): Medicinal Chemistry and Synthesis of Selective Drugs / Advanced Inorganic Chemistry / Computational Chemistry and Numerical Analysis / Principles and applications of electrochemistry	3	0	0	3	3	100
3	CH6271	M.Sc Thesis Part-II	0	0	16	16	8	200
4	CH6291	Thesis Seminar & Viva voce	0	0	0	0	4	100
<b>Total</b>			<b>6</b>	<b>1</b>	<b>16</b>	<b>23</b>	<b>19</b>	<b>500</b>

**\*\*Chemistry Department offers three specializations (Physical /Inorganic/ Organic)  
Total Credits = [22+28+23+19]= 92; Total Marks = 600 + 800 + 600 + 500 = 2500.**

## SEMESTER I

### CH5101: Quantum mechanics and molecular spectroscopy

- 04 Credit

#### Unit 1: Basic Quantum Mechanics

24 L

Basic postulates of quantum mechanics, Generalized uncertainty principle, Time evaluations of the system's states, Stationary states: Time-independent potentials, Properties of one, two and three dimensional problems (particle in a box, on a ring and on a sphere), Angular momentum, Harmonic Oscillator (wavefunction and operator methods), Barrier and tunneling problems,

#### Reference Books:

- 1) Introduction to Quantum Mechanics by L. Pauling and E. B. Wilson
- 2) Molecular Quantum Mechanics by P. Atkins
- 3) Elementary Quantum Chemistry by F. L. Pilar
- 4) Quantum Mechanics by J. L. Powell and B. Crasemann
- 5) Introduction to Quantum Mechanics by D. J. Griffiths
- 6) Principles of Quantum Mechanics by R. Shankar
- 7) Quantum Mechanics: Concepts and Applications by N. Zettili
- 8) Introductory Quantum Mechanics by R. Liboff
- 9) Quantum Mechanics by Claude Cohen-Tannoudji
- 10) Physical Chemistry : A Molecular Approach – D. A. McQuarrie and J. D. Simon
- 11) An Introduction to Quantum Mechanics by P. T. Matthews
- 12) Quantum Mechanics in Chemistry by G. C. Schatz and M. A. Ratner

#### Unit 2: Spectroscopy

24 L

Theory of absorption and emission (spontaneous and stimulated) of light; symmetry operations; origin of selection rules and use of group theory; rotational, vibrational (Raman and IR) and electronic spectroscopy; Franck-Condon factor and processes in representative Jablonski diagram, theory and representative techniques in time- and polarization-resolved spectroscopy; working principle of optics and short-pulse generation. Introduction to magnetic spectroscopy.

#### Reference Books:

- 1) Symmetry & Spectroscopy, Bertoluchi & Harris
- 2) Molecular Spectroscopy, Banwell
- 3) Molecular Spectroscopy, Hollas
- 4) Molecular Spectroscopy, I Levine

### CH5102: Transition metal chemistry: Structure-bonding correlation, Magnetic properties and Bioinorganic Chemistry

- 04 Credit

#### Unit 1: Spectra and bonding in transition metal complexes

24L

Crystal-Field Theory, Term Symbols, microstates, R-S coupling, Free ion terms, Inter-electronic Repulsion Parameters, Splitting of Free ion terms under crystal field potential, Correlation Diagram, Hole formalism, inversion and equivalence relations, Orgel Diagrams (qualitative approach), Qualitative idea of Tanabe-Sugano Diagrams, Selection Rules of Electronic Transition: Laporte Forbidden Rule, Spin Selection Rule, Electronic spectroscopy of Transition Metal Complexes, Characteristic spectra of octahedral, tetrahedral and square planar complexes of transition metal ions, Effect of Tetragonal Distortions.

Molecular Orbital Theory (MOT): Symmetry adapted linear combination of AOs to construct MOs of simple molecules, Shape of molecules – construction of hybrid orbital using molecular symmetry, Walsh diagram; Evidence of MO pictures from spectra and reactivity, The concept of a Ligand field, Scope of ligand field theory, MO description of Transition Metal complexes in Octahedral, Tetrahedral & Square Planar

Geometric arrangements, Spectrochemical and Nephelauxetic series, Charge Transfer Spectra (CT), Ligand to Metal Charge Transfer (LMCT), Metal to Ligand Charge Transfer (MLCT), Ligand to Ligand Charge Transfer (LLCT)

**Reference Books:**

- 1) Ligand Field Theory – B.N. Figgis
- 2) Electronic Structure and Properties of transition metal compounds – I.B. Bersuker
- 3) Ligand Field Theory – C.J. Ballhausen
- 4) Electronic Absorption Spectroscopy – D.N. Satyanarayana
- 5) Inorganic Electronic Spectroscopy – A.B.P. Lever

**Unit 2: Magnetochemistry**

**12L**

Definition of magnetic properties, Types of magnetic bodies, Experimental arrangements for the determination of magnetic susceptibility: Guoy method, Faraday method, Vibrating sample magnetometer, SQUID, NMR method; Anisotropy in magnetic susceptibility, diamagnetism in atoms and polynuclear systems, Pascals constant, Two sources of paramagnetism: Spin & Orbital effects, Spin orbit coupling, Lande interval rule, Energies of J levels, Curie equation, Curie & Curie – Weiss law, First order & second order paramagnetism, Temperature independent paramagnetism, Simplification & application of Van Vleck susceptibility equation, Quenching of orbital moment, Magnetic behaviour of lanthanides & actinides, Lose spin – high spin cross over.

**Reference Books**

- 1) Magnetochemistry – R.L. Dutta and A. Syamal
- 2) Magnetochemistry – F.E. Mabbs and D.J. Machine

**Unit 3: Bio-inorganic chemistry**

**12L**

Elements of life, the natural selection of elements, metallo-biomolecules– enzymes and proteins, their differences, homeostatis and detoxification, Metal ion storage and transport : Ferritin, metallothioneins, cerruloplasmin, Vanadium storage in tunicates and ascidians; Siderophores – enterobactin, transferrin; Natural Oxygen carriers : Hemoglobin, Hemocyanin, Hemerythrin– model compounds. Hydrolytic enzyme: CarboxypeptidaseA, Redox enzyme: Blue Copper protein.

**Reference Books**

- 1) Bioinorganic Chemistry – I. Bertini, H.B. Gray, S.J. Lippard, J.S. Valentine.
- 2) Bioinorganic Chemistry – S.J. Lippard and J.M. Berg
- 3) Bioinorganic Chemistry – W. Kaim & G. Schroedder
- 4) Inorganic Biochemistry– J. A. Cowan

**CH5103: Stereochemistry, Reaction Mechanism and Heterocyclic Chemistry - 04 Credit**

**Unit 1: Stereochemistry**

**24L**

Static Stereochemistry: Symmetry, point group, ligand and face topicity, chirality, molecules with more than one chiral centres straight chain or branched. Optical activity in absence of chiral carbon (biphenyls, allenes and spirans). Chirality due to helical shape. Stereochemistry of compounds containing N, S, P. Curtin-Hammett principle, Conformational analysis of cyclohexane, cyclohexene, cyclohexanone, decalin and their derivatives; perhydroanthracene, perhydrophenanthrene,  $\alpha$ -strain,  $\beta$ -strain, allylic 1,2 and 1,3-strain.

Dynamic Aspects: Prelog's rule, Cram's rule, Karabatsos's rule, Felkins rule and their applications in organic synthesis, Felkin-Anh, Cieplak and Zimmerman-Traxler Models; Asymmetric Synthesis: Enantio- and diastereoselective synthesis, Addition to carbonyl compounds: use of chiral substrate, chiral reagent, chiral catalyst; Addition to C=C double bonds, Reduction of C=C double bonds, Stereoselective reactions of carbonyl compounds: Reactions of enolates ( $\alpha$ -substitution), alkylation, asymmetric aldol reactions; stereoselective hydrogenation, epoxidation, hydroxylation, aminohydroxylation, cyclopropanation.

**Reference Books:**

- 1) Stereochemistry of Carbon Compound – E.L. Elien

- 2) Stereochemistry of Organic Compound – D. Nosipuri
- 3) Stereochemistry of Organic Compounds -E. L. Eliel and S. H. Wilen
- 4) G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001
- 5) Organic Mechanisms: Reactions, Stereochemistry and Synthesis R. Bruckner, (Springer)

### Unit 2: Organic Reaction Mechanism

12 L

Physical organic chemistry: Preliminary ideas on quantitative correlation of rates and equilibria, Kinetic and thermodynamic control of product formation, Reaction coordinate diagram, Transition state (activated complex), Principle of microscopic reversibility, Hammond's postulate, Linear free energy relationships with special reference to the Hammett equation and related modifications, Catalysis (acids, bases, and nucleophilic) and isotope effects.

Reactive intermediates: Formation, stability and reactivity of carbocations, carbanions (classical and non-classical), carbenes, nitrenes, arynes and free radicals with reference to basic types of organic reactions, typical examples of substitution, elimination and addition reactions.

#### Reference Books:

- 1) Advanced Organic Chemistry – Jerry March
- 2) Some Modern methods of Organic Synthesis – W. Carruthers
- 3) Advanced Organic Chemistry – F.A.Carey & R.J. Sundberg
- 4) Mechanisms and Theory in Organic Chemistry, T. H. Lowry and K. H. Richardson,
- 5) Advance Organic Chemistry: Reaction Mechanisms, B. Reinhard (Elsevier).

### Unit 3: Heterocyclic Chemistry

12 L

Nomenclature and classification of heterocycles structure.

Synthesis and reactivity of a) 5,6-membered rings containing two or more heteroatoms (pyrazole, imidazole, oxazole, thiazole, isooxazole and their benzo derivatives, triazole, pyrimidine, pyridazines, pyrazines, coumarins, chromones, purines and pteridines); b) Introduction to the chemistry of seven-membered heterocyclic compounds: azepines, oxepines, thiepinines; c) Heterocyclic systems containing Phosphorous and selenium, Application of heterocycles in pharmaceutical and electronic industry (conjugated molecules).

#### Reference Books:

- 1) Heterocyclic Chemistry – J.A. Joule & K. Mills
- 2) Heterocyclic Chemistry – J.A. Joule & G.F. Smith
- 3) Heterocyclic Chemistry – R.K. Bansal.
- 4) Palladium in Heterocyclic Chemistry: A Guide for the Synthetic Chemist, Li, J. J. & Gribble, G.W.
- 5) Heterocyclic Chemistry, T. L. Gilchrist, (Pearson Education).
- 6) Handbook of Heterocyclic Chemistry. Alan R. Katritzky and A. F. Pozharskii, (Elsevier).
- 7) Topics in Heterocycles Chemistry. G. W. Gribble. (Spinger).
- 8) Modern Heterocyclic Chemistry.4 Volume Set. Julio A.-B., Juan Jose Vaquero, José Barluenga. (Wiley).

## CH5121: Group Theory and Application of Spectroscopy

- 03 Credit

### Unit 1: Group theory

12 L

Definitions and theorems of group, subgroup, class, Symmetry operations and symmetry elements, Point groups, physical properties: Polarity, Chirality etc., Matrix representations of symmetry operations, group multiplication, Properties of matrix representations: Similarity transforms, Characters of representations, Irreducible and reducible representations of group, the Great Orthogonality Theorem, character tables.

#### Reference Books:

- 1) Chemical Applications of Group Theory by F.A.Cotton; Wiley.
- 2) Molecular Symmetry and Group Theory by Robert L. Carter; Wiley.



**Unit 2: Application of Spectroscopy in Organic Chemistry****12 L**

IR Spectroscopy: Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic and heterocyclic compounds, ethers, phenols and amines, carbonyl compounds (aldehydes, ketones, esters, carboxylic acids, amides, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effects of solvent, hydrogen bonding on vibrational frequencies, overtones, combination bands and Fermi resonance.

Mass spectrometry: Instrumentation, Mass spectral fragmentation of organic compounds, McLafferty rearrangement, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Nuclear magnetic resonance ( $^1\text{H}$  &  $^{13}\text{C}$  NMR): Factors affecting nuclear relaxation, chemical shift, spin-spin interaction, shielding mechanism, complex spin-spin interaction, Karplus curve, variation of coupling constant with dihedral angle, nuclear magnetic double resonance, simplification of complex spectra, chemical shift reagent. Introduction  $^{13}\text{C}$  NMR. Structure determination using combined spectroscopic methods.

**Reference Books**

- 1) Organic Spectroscopy – W. Kemp
- 2) Introduction to Organic Spectroscopy – L.K. Pavia, Lampman and Kriz
- 3) Spectrometric Identification of Organic Compounds – R. M. Silverstein, G. C. Bassler and T. C. Morrill
- 4) Organic Spectroscopic Analysis – R.J. Anderson, D.J. Bendelm & P.W. Groundwater

**Unit 3: Application of Spectroscopy in Inorganic Chemistry****12L**

FT-IR of Transition metal Complexes containing CO, NO, CN<sup>-</sup>, SCN<sup>-</sup>, ClO<sub>4</sub><sup>-</sup>, NH<sub>2</sub><sup>-</sup>etc group. Raman Spectra: Classical Theory, Quantum Theory, Rotational Raman, Vibrational Raman & Resonance Raman spectroscopy, Basic principle and application of CD, ORD and MCD.

**Reference Book:**

- 1) Handbook of Molecular Spectroscopy – D. N.Sathyanarana,
- 2) Practical Raman Spectroscopy: An Introduction– Peter Vandenabeele
- 3) Physical Methods for Chemists–Russell S. Drago
- 4) ORD and CD in Chemistry and Biochemistry: An Introduction–Pierre Crabbe

**CH5122: Instrumental Techniques for Chemical Analysis****- 03 Credit****Unit 1: Mathematical Methods in Chemistry****12L**

Elements of Differentiation & Integration, Differential Equations, Extremum principles, Constrained extremization, Power series: Convergence & divergence, Taylor, Maclaurin & Fourier series, Fourier Transforms, Delta & Gamma functions, Fundamentals of Linear Algebra, Probability density function (Definition, Formula & Example).

**Reference Books**

- 1) D. A. McQuarrie and M. Hansen, Mathematics for Physical Chemistry, University Science Book.
- 2) M. L. Boas, Mathematical methods for the physical sciences, Kaye Pace, Ed. 3<sup>rd</sup>.
- 3) P. G. Francis, Mathematics for Chemists, Springer.
- 4) J. Matthews and R. L. Walker, Mathematical methods of physics, Addison Wesley Longman, Ed. 2<sup>nd</sup>.
- 5) G. Arfken, H. Weber and F. Harris, Mathematical methods for physicists, Academic Press, Ed. 7<sup>th</sup>.
- 6) I. Savov, No Bullshit Guide to Math and Physics, Minireference Co.; 5<sup>th</sup> edition.
- 7) E. Kreyszig Advanced Engineering Mathematics, Wiley.
- 8) D. Z. Goodson, Mathematical Methods for Physical and Analytical Chemistry, Wiley-Blackwell.

**Unit 2: Thermal methods and Atomic spectroscopies****12L**

Thermal analysis (TG, DTA & DSC): Instrumentation and application, Factors affecting the Thermal Analysis Curves. Atomic emission, Atomic absorption and Atomic fluorescence spectrometry

**Reference Books**

- 1) Fundamentals of Analytical Chemistry –Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch,
- 2) Instrumental Methods of Analysis– Hobart H. Willard, Lynne L. Merritt, Jr.; John A. Dean

**Unit 3: Instrumental Techniques for organic based materials****12L**

Details of instrumentation, principles and applications of UV, IR, NMR, GC, GC-MS, HPLC, GPC, XRD, Fluorometer for synthetic.

**Reference Books**

- 1) Fundamentals of Analytical Chemistry –D.A. Skoog, D. M. West, F. James Holler, S. R. Crouch,
- 2) Vogel's Text Book of Practical Organic Chemistry (**Vol 2**)– A.R. Tatchell
- 3) Introduction to Organic Laboratory technique – Pavia, Lampman, Kriz & Engel
- 4) Organic Experiments – K.L. Williamson
- 5) General Chemistry Experiments – A.J. Elias

**CH5261: Chemistry of nanomaterial****- 03 Credit****Unit 1: Basic understanding and synthesis of nanomaterials:****12L**

Definition of Nano, Scientific revolution- Atomic Structure and atomic size, emergence and challenges of nanoscience and nanotechnology, carbon age-new form of carbon (CNT to Graphene), influence of nano over micro/macro, size effects and crystals, large surface to volume ratio, surface effects on the properties, different synthesis methods for the preparation of nanomaterials: Solution, Hydrothermal, Sonochemical, Micro-wave assisted, CVD, Sol-emulsion-gel method.

**Unit 2: Physical aspects and application****24L**

**Physical aspects:** One dimensional, two dimensional and three dimensional nanostructured semiconductor materials: band-diagram, density of states, Fermi level and carrier concentration, absorption spectrum, properties of nanodimension Quantum dots shell structures; metal nanoparticles, Mie theory and simulation methods, localized surface plasmon resonance, plasmon lifetime, plasmon hybridization

**Application:** photovoltaic, light emitting diodes, semiconductor laser, application of plasmonics, metal-semiconductor hetero-structure, biological and environmental, membrane based application, polymer based application.

**Reference Books**

- 1) Plasmonics: fundamentals and applications, Steve Maier
- 2) Electronic properties of crystalline solids, R. H. Bube
- 3) Semiconductor optics, C. Klingshirn
- 4) Nanostructures and Nanomaterials- G. Cao, Y. Wang
- 5) Nanoscale materials in chemistry-Kenneth J Klabunde, Ryan M Richards

**CH5171: Inorganic Chemistry Laboratory-I****- 02 Credit**

Synthesis and characterization of isomers of nitro and nitrito pentaamine Cobalt(III) complexes *cis* and *trans*  $[\text{Co}(\text{NH}_3)_4\text{Cl}_2]\text{NO}_3$ : Synthesis and characterization

Preparation and characterization of  $\text{K}_3[\text{Cr}(\text{O}_2)_4]$

Preparation of  $[\text{Co}(\text{NH}_3)_4\text{CO}_3]\text{Cl}$ ,  $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$  and  $[\text{Co}(\text{NH}_3)_5\text{N}_3]\text{Cl}_2$ , IR and Electronic spectra and solution conductance of these compounds.

Preparation of  $\text{Fe}(\text{salen})_2\text{O}$  and estimation of iron in the sample. Characterization of the compound by IR Electronic spectra and Magnetic moment measurement.

A chemical bath deposition technique for the deposition of thin film semiconductors

Preparation of Co(salen) and [(py)(salen)Co-O-O-Co(salen)(py)] and study of their Electronic and IR spectra and analysis of their Cyclic- voltammograms.

Tetraphenyl porphyrine complexes of Cu(II), Ni(II), Zn(II) and Fe(III): Characterization of the compound by IR Electronic spectra and Magnetic moment measurement

Synthesis and Characterization of VO(acac)<sub>2</sub> and Mn(acac)<sub>3</sub>

### **CH5172: Organic Chemistry Laboratory-I**

**- 02 Credit**

**Qualitative analysis:** Separation, purification and identification of compounds of binary mixture using TLC and column chromatography, chemical tests.

**Organic synthesis:** Oxidation reaction: Benzaldehyde by PCC oxidation of benzyl alcohol or adipic acid by chromic acid oxidation of cyclohexanol.

Aldol condensation: Dibenzal acetone from benzaldehyde.

Friedel Crafts reaction:  $\beta$ -Benzoyl propionic acid from succinic anhydride and benzene.

#### **Reference Books:**

- 1) Vogel's Text Book of Practical Organic Chemistry – A.R. Tatchell
- 2) Introduction to Organic Laboratory technique – Pavia, Lampman, Kriz & Engel
- 3) Organic Experiments – K.L. Williamson
- 4) General Chemistry Experiments – A.J. Elias
- 5) Comprehensive Practical Organic Chemistry – V.K. Ahluwalia & R Agarwal

## SEMESTER II

### **CH5201: Classical and statistical thermodynamics, surface and bio-physical chemistry - 04 Credit**

#### **Unit 1: Classical thermodynamics**

**12 L**

Thermodynamic properties of gases with special reference to ideal and real gases and their mixtures. Thermodynamics of ideal and non-ideal binary solutions, Partial molar properties, mixing quantities & excess functions for non-ideal solutions and their determination. Gibbs Duhem equation applied to activity coefficient (osmotic coefficient). Different scales of activity coefficients for solutions and solvents. Experimental determination of activity coefficients of electrolytes and non electrolytes, forces & fluxes, concepts of entropy productions, penomenological coefficient, Onsager reciprocal relations and their applications.

#### **Reference Books:**

- 1) Physical Chemistry, I R Levine
- 2) Physical Chemistry a Molecular Approach, Donald A. McQuarrie and John D. Simon
- 3) Molecular Thermodynamics, Donald A. McQuarrie and John D. Simon.

#### **Unit 2: Statistical mechanics/thermodynamics**

**12 L**

Introduction, scope, limitations of conventional thermodynamics and purpose of statistical thermodynamics. Statistical concepts and examples. Basic postulates (only statements); Entropy and probability. Thermodynamic properties in dilute limit; thermodynamic properties from partition function; Equipartition theorem and its applications: Specific heats of solids, Maxwell velocity distribution. Equilibrium conditions and constraints. Reversible and irreversible processes; Distribution of energy between systems in equilibrium. System in contact with heat reservoir; Gibbs paradox; Sackur–Tetrode equation; Validity of the classical approximation; Information theory.

#### **Reference Books:**

- 1) Fundamentals of Statistical and Thermal Physics, F. Reif
- 2) Statistical thermodynamics, N. M. Laurendeau
- 3) Equilibrium Statistical Mechanics, E. A. Jackson
- 4) The Principles of Chemical Equilibrium, K. Denbigh

#### **Unit 3: Surface Chemistry**

**12 L**

Adsorption isotherms: Freundlich, Langmuir, BET. Adsorption on porous solids. Chemisorption of gases on solid surface. Kinetics of adsorption processes, Heterogeneous catalysis. Characterization of solid surface structure and composition using different techniques. Spreading coefficient of liquid.

#### **Reference Books:**

- 1) Physical Chemistry by S. Galsstone
- 2) Physical Chemistry by G. W. Castellan
- 3) Physical Chemistry by McQuarrie and Simon; Viva

#### **Unit 4: Biophysical Chemistry**

**12 L**

Introduction of structure of Bio-molecules. Membrane structure, ion Channels. Bio-molecular complexes. Stabilizing interactions of macromolecules. Simulating macromolecular structure. Statistical models for structural transitions in macromolecules: All or none, non-cooperative, zipper. Non-regular structure: Random walk and Simple exact models. Chemical equilibrium involving binding of small ligand by macromolecules. Structural determination of bio-molecules.

#### **Reference Books:**

- 1) Biochemistry, by Berg, Tymoczko, Stryer; MacMillan
- 2) Principles of Physical Biochemistry, by Holde, Johnson, Ho; Prentice Hall
- 3) Physical chemistry: Principles and Applications in Biological Sciences by Tinoco, Sauer, Wang, Puglisi, Harbison, Rovnyak; Pearson

## CH5202: Organometallic, Homogeneous catalysis and Solid state chemistry - 04 Credit

### Unit 1: Organometallic Chemistry

12L

Introduction, Classical and non-classically bonded organometallic compounds, Metal-olefin complexes, Ziese's salt – modes of bonding, Non-conjugated and conjugated polenyl complexes and their bonding models specially allyl derivatives, Metal complexes of delocalised carbocycles, Metallocenes and metal arenes, Ferrocene, ruthenocene – structure and bonding , reactions. Multidecker compounds. Fluxional behavior of organometallic compounds. Transition metal carbene complexes, oxidative addition and migration (Insertion reaction ).

### Unit 2: Homogeneous Catalysis

12L

Introduction to catalysis, Catalysis by organometallic compounds: Alkene hydrogenation (including asymmetric hydrogenation), Wilkinson Catalyst, Tolman catalytic loops, synthetic gas, water gas shift reactions, synthesis of methanol, hydroformylation ( oxo process ), hydrosilation of unsaturated compounds, Monsanto acetic acid process, Walker process, Hydrocyanation of alkenes, Synthetic gasoline, Fischer Tropsch and Mobil process, oligomerisation, polymerisation and metathesis reactions of alkenes and alkynes, Ziegler Natta Catalysis.

### Reference Books :

- 1) Organometallic Chemistry – R.C. Mehrotra and A. Singh
- 2) Organometallic Chemistry – R.H. Crabtree
- 3) Organometallic Chemistry – M. Bochmann (Oxford series)

### Unit 3: Electronic properties of materials, Crystal Structure and Defects

12L

Evolution of band structure, Brillouin zone, Effective mass of electron, Energy spectrum of electrons in a crystal, Occupation of bands by electrons, Intrinsic semiconductors, Concept of hole, Extrinsic semiconductors, Carrier mobility, Hall effect, Electrical conductivity of metals, alloys & semiconductors, Degenerate & Nondegenerate ensembles, Fermi levels in metals & semiconductors, Direct & indirect band gap semiconductors, Photo-conductivity

Simple type structures: Sphalerite, Wurtzite, Halite, Nicolite, Fluorite, Antifluorite, Rutile, CdCl<sub>2</sub>, CdI<sub>2</sub>, Spinel, Perovskite, Silicate

Defects: i) Point defects: Schottky, Frenkel, Colour centres, Vacancies & interstitials in non-stoichiometric crystals, Defect clusters, Order-disorder phenomena, Solid solutions,

ii) Line defects: Edge dislocation, Screw dislocation, Dislocation loops

iii) Plane defect: Crystallographic shear structures, Stacking faults, Sub-grain boundaries & Anti-phase domains

### Unit 4: Solid state reactions and introduction to nanochemistry

12L

Type I and Type II reactions, Polymorphism, Enantiotropy & Monotropy, Martensitic Transformations, Order-disorder transitions, Polytypism, Sintering, Zone refining, Crystal growth, Growth from solutions, Flame fusion method, Vapour deposition technique, Chemical transport reaction, Growth by condensation.

Theoretical aspects; preparation, characterization, and applications of nanomaterials. Properties of nanomaterials and nanoparticles.

### Reference Books

- 1) The Structure & Properties of Materials – J. Wulff & Wiley, Vol – IV.
- 2) Electronic Properties of Materials – R.E. Hummel & Springer
- 3) Introduction to Solids – L.V. Azaroff
- 4) Basic Solid State Chemistry – A.R. West & Wiley
- 5) Solid State Chemistry – D.K. Chakraborty
- 6) Solid State Physics – A.J. Dekker
- 7) Introduction to Solid State Physics – Charles Kittel

**Unit 1: Modern Reagents for Organic Synthesis****12 L**

Lithium diisopropylamide (LDA), Organoboron chemistry: Hydroboration, regio-, chemo- and stereoselectivity. Conversion of C-B bond to C-hetero and C-C bonds, Use of allylboration and crotylboration. Chemistry of organosilicon compounds: Synthetic uses of silyl ethers, silylenol ethers, TMSCN, trimethylsilyl iodide, alkynyl, vinyl, aryl, allyl and acyl silanes; Organophosphorous chemistry: phosphorus ylides, Wittig reaction and its modifications. Chiral Phosphines and phosphites. Arbutov reaction. Organosulfur and selenium chemistry: application of sulphoxides, sulfones and sulphur ylides in organic synthesis, Gilman's reagent (organocopper reagents), organoaluminum compounds, Organochromium reagents, Organotin reagent.

**Unit 2: Selective Name Reactions****12 L**

Shapiro reaction, Peterson olefinations, Robinson annulation, Mitsunobu reaction, Hofmann-Löffler-Freytag reaction, Barton reaction, Mukayama-aldol reaction, Evans' Aldol reaction, Baylis-Hillman reaction, Henry reaction, Kulinkovich reaction, Tebbe olefination, Ritter reaction, Nef reaction, Sakurai reaction, Brook rearrangement.

**Unit 3: Concepts in organic synthesis****12L**

Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups. Designing synthesis of some target molecules with proper retrosynthetic analysis: e.g. Menthol, acyl anion equivalent, protection of carbon-carbon multiple bonds, protection and deprotection in synthesis.

Baldwin rules and exceptions, Different approaches towards the synthesis of three, four, five, and six-membered rings, Pauson-Khand reaction, Bergman cyclization, Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization, inter-conversion of ring systems (contraction and expansion).

**Unit 4: Oxidation and Reduction****12 L**

Metal based and non-metal based oxidations of alcohols (chromium, manganese, silver, ruthenium, DMSO, and hypervalent iodine etc); Peroxides oxidation of alkenes and carbonyls; Alkenes to diols (manganese, osmium based), alkenes to carbonyls with bond cleavage (manganese, ruthenium, and lead based, ozonolysis), and alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, and selenium based allylic oxidation); Asymmetric epoxidations (Sharpless, Jacobsen, and Shi epoxidations).

Catalytic homogeneous and heterogeneous hydrogenation, Wilkinson catalyst; Reductions by dissolving metals, Li/Na in liquid ammonia, zinc, titanium, and samarium; Hydride transfer reagents: NaBH<sub>4</sub>, L-selectride, K-selectride, Luche reduction, LiAlH<sub>4</sub>, DIBAL-H, Red-Al, Trialkylsilanes; Reduction by Bu<sub>3</sub>SnH/AIBN; Enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata) and Noyori asymmetric hydrogenation; Baker yeast.

**Reference Books:**

- 1) Organic Synthesis – The Disconnection Approach – S. Warren
- 2) Principle of organic synthesis -R.O.C. Norman & J. M. Coxon
- 3) Organometallic Chemistry – R.C. Mehrotra & A. Singh
- 4) Organometallic Chemistry – L.S. Hege
- 5) Modern methods of Organic Synthesis – W. Carruthers
- 6) Advanced Organic Chemistry – F.A. Carey & R.J. Sundberg
- 7) Named Organic Reactions – T. Laue & A. Plagens
- 8) Applications of named Reactions in Organic Synthesis, Kuerti and B. Czako, Strategic, (Elsevier)
- 9) Organic Chemistry, Clayden, N. Greeves, S. Warren and P. Wothers, (Oxford University Press).
- 10) Advanced Organic Chemistry, A. Carey and R. I. Sundberg, Part A and B, (Springer).
- 11) Organic Synthesis, The disconnection Approach, Warren, (John Wiley & Sons).
- 12) Catalytic Asymmetric Synthesis, Ojima, (Wiley-VCH)
- 13) Asymmetric Catalysis in Organic Synthesis, Noyori, (Wiley & Sons)

## CH5221: Green Chemistry, Pericyclic Reactions and Organic Photochemistry - 03 Credit

### Unit 1: Green Chemistry

12 L

Green Chemistry definition, need for Green chemistry, evolution of Green Chemistry, basic principles of Green Chemistry.

Classification of organic reactions under Green chemistry principles: a) Atom economic and non-toxic byproduct reactions: rearrangements, addition reaction, condensations, cascade strategies under catalysis, b) atom uneconomic reactions: substitutions, eliminations, Wittig reactions, degradation reactions

Green Strategies and techniques for Organic Synthesis: use of Microwave, Ultrasound assisted reactions, Ball mill technique, and photochemical reactions

Catalysis: Principles of various catalysis techniques in terms of Green Organic Synthesis i) Homogeneous, ii) Heterogeneous, iii) bio (enzyme) catalysis, iv) catalysis with nontoxic metals (Ca, Fe, Co, etc.), v) solid supported catalysis, vi) metal free/organocatalysis, vii) Visible light catalysis viii) phase transfer catalysis

Alternative/Green Solvents for Organic Synthesis i) Water, ii) Ionic liquids, iii) Supercritical liquids (SCL), iv) Poly(ethylene glycol) (PEG), v) Fluorous biphasic Solvents

Solvent Free Organic Synthesis, Reactions at Room Temperature, Multicomponent reactions (Ugi Reaction, Biginelli reaction, etc...), Applications of Green Chemistry to Chemical Synthesis.

#### Reference Books:

- 1) Green Chemistry: Theory and Practice – Paul T. Anastas & John C. Warner
- 2) New Trends in Green Chemistry – V. K. Ahluwalia & M. Kidwai
- 3) Green Chemistry 1st Edition – Bela Torok & Timothy Dransfield
- 4) Handbook of Green Chemistry and Technology – James H. Clark & Duncan Macquarrie
- 5) Green Organic Chemistry in Lecture and Laboratory – Andrew P. Dicks
- 6) Strategies for Green Organic Synthesis, by V. K. Ahulwalia,.
- 7) Green Chemistry: An introductory text book by Mike Lancaster, RSC publication
- 8) Green Chemistry: Environmental friendly alternatives by Rashmi Sanghi and M M Srivastava,

### Unit 2: Pericyclic Reactions

12 L

Introduction to pericyclic reactions, Woodward–Hoffmann rule, Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions (electrocyclic, sigmatropic, cycloaddition and ene reactions). Selection rules and stereochemical aspects of electrocyclic reactions, cycloaddition and sigmatropic shifts. Electrocyclic reactions: conrotatory and disrotatory motions,  $4n$ ,  $4n+2$  and allyl systems. Cycloaddition reactions: antarafacial and suprafacial additions,  $4n$  and  $4n+2$  systems; 2,2 addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3, 3- and 5,5- sigmatropic rearrangements. Cope, Claisen, oxy-Cope and aza-Cope rearrangements. Ene reaction. Orbital coefficient, energy diagram of different substituted ethylene and butadiene systems. Study of cycloaddition reaction using different substituted ethylene and butadiene systems by considering Regioselectivity, Periselectivity, Site selectivity and Secondary orbital interactions.

#### Reference Books:

- 1) Pericyclic Reaction Vols. I & II - R.E. – Lehr & A. P. Marchand.
- 2) Pericyclic Reaction – S.M. Mukherjee
- 3) Photochemistry & Pericyclic Reactions, J. Singh & J. Singh,
- 4) Frontier Orbitals and Organic Chemical Reactions, I. Fleming, (Wiley).
- 5) Conservation of Orbital Symmetry, B. B. Woodward and Hoffman,
- 6) Organic Synthesis, M. Smith, (Mc Graw Hill),

### Unit 3: Organic Photochemistry

12 L

Singlet and triplet excited state, Radiative and radiationless transition, Potential energy surfaces, Classification of reaction types, Molecular rearrangements and fragmentation reactions, Excimers and

exciplexes. Photochemistry of olefins and carbonyl compounds, photo oxygenation and photo fragmentation, Photochemistry of aromatic compounds: isomerisation, Additions and substitutions. Singlet molecular oxygen reactions. Paterno-Buchi reaction, Di-pimethane rearrangement, Bartons reaction and Photo-Fries Photochemistry of alkenes, carbonyl, aromatic compounds, miscellaneous photochemical reactions.

**Reference Books:**

- 1) Organic Photochemistry – J. Coxon & B. Halton
- 2) Introductory Photochemistry – A. Cox & T. Camp

**CH5222: Photophysical processes and polymer chemistry**

**- 03 Credit**

**Unit I: Photophysical processes**

**24 L**

Violation of selection rules (spin orbit coupling, vibronic coupling); fluorescence and phosphorescence, delayed fluorescence; properties of electronically excited molecules: lifetime (relation with quantum yield), redox potential, dipole moment, pK values. Fluorescence quenching (dynamic and static) mechanisms: energy transfer, electron transfer (Marcus theory, Rehm-Weller theory), proton transfer, complex formation phenomenon (excimer, exciplex) in excited state; decay kinetics of photo-physical processes. Emission and excitation anisotropy; photo-catalysis; molecular design and electronic spectra, time-resolved spectroscopy for reaction mechanism.

**Reference Books:**

- 1) Photophysics of aromatic molecules: J. B. Birks
- 2) Principles of fluorescence spectroscopy, J. R. Lakowicz.
- 3) The theory of the electronic spectra of organic molecules, J. N. Murrell
- 4) Modern Molecular Photochemistry, N. J. Turro

**Unit 2: Polymer chemistry**

**12 L**

Introduction and applications of polymers, molecular weight distributions, various experimental methods (GPC/SEC, solution viscosity, VPO, light scattering) to determine relative and absolute molecular weight distributions, chain growth and step growth mechanisms and kinetics, ionic polymerization, living polymerization, stereochemistry of polymers, free radical copolymerization (random, block, alternate and graft copolymers), kinetics and mechanisms of free radical copolymerization, polymerization conditions and polymer reactions, thermal, mechanical and solution properties of polymers, thermoplastics, thermosets and elastomers, conducting polymers, branched polymers (star, dendritic and hyperbranched polymers).

**Reference Books:**

- 1) Hand Book of Polymer Science & Technology – M.H. Ferry & A.V. Becker
- 2) Text Book of Polymer Chemistry – F.W. Billmeyer.
- 3) Principles of Polymer Chemistry - Paul J. Flory.
- 4) Conducting Polymers: A New Era in Electrochemistry, György Inzelt.



## CH5223: Advanced bioinorganic and inorganic supramolecular chemistry - 03 Credit

### Unit 1: Advanced Bio-inorganic chemistry

12L

Oxygen management: Super oxide dismutase, catalase, peroxidase, cytochrome P-450. Chemistry of Vitamin B<sub>12</sub>, Iron – Sulphur proteins, Cytochrome, Metal toxicity and Chelation therapy, Nitrogenase-biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidences, other nitrogenase model systems, Bioenergetics and ATP cycle: DNA polymerization, glucose storage, metal complexes in transmission of energy, chlorophylls, Photosystem I and II in cleavage of water- Model systems; Na<sup>+</sup>, K<sup>+</sup> pump, Ca<sup>2+</sup> transport.

### Unit 2: Bio-inspired approach in Inorganic Chemistry

12L

Approach to molecular Design, Synthesis of functional and structural model complexes of natural enzymes, characterization and possibilities for Application. Metal ions and metal complex interactions with nucleic acid and DNA: Coordination, Intercalation and hydrogen bonding.

Nanozymes: Concept of Artificial Enzymes, Mechanism and Application

Metal organic frameworks mimicking natural enzymes: Structural and Functional correlation

### Unit-3: Molecular Recognition and Inorganic Supramolecular Chemistry

12L

Concept of supramolecular chemistry, supramolecular building blocks and spacers, molecular recognition and host-guest interaction, molecular receptors for different types of ions and molecules. Ditopic and polytopic receptors, metal assisted molecular and supramolecular assemblies. Anion Co-ordination chemistry, Supramolecular ionic and switching devices, Molecular wires, molecular sensors and switches, molecular machines; molecular electronics. Concept of biosensor.

#### Reference books:

- 1) Bioinorganic Chemistry – I. Bertini, H.B. Gray, S.J. Lippard, J.S. Valentine.
- 2) Bioinorganic Chemistry – S.J. Lippard and J.M. Berg
- 3) Bioinorganic Chemistry – W. Kaim & G. Schroedder
- 4) Supramolecular Chemistry– J.W. Steed and J. L. Atwood
- 5) Anion Coordination Chemistry–A. Bianchi, K. Bowman-James, E. García-España
- 6) Molecular devices and machines– V. Balzani

## CH5261: Spectroscopy for Chemical Analysis

- 03 Credit

### Unit 1: Spectroscopic analysis for organic compounds

24L

UV-VIS Spectroscopy: Various electronic transitions (185-800 nm), effect of solvent, Lambert-Beer law; uv-bands of saturated and unsaturated carbonyl compounds, -dienes, -conjugated polyenes, Fieser-Woodward rules; IR Spectroscopy: Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic and heterocyclic compounds, ethers, phenols and amines, carbonyl compounds (aldehydes, ketones, esters, carboxylic acids, amides, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effects of solvent, hydrogen bonding on vibrational frequencies, overtones, combination bands and Fermi resonance. Nuclear magnetic resonance (<sup>1</sup>H NMR only): Basic instrumentation, nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift, and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification of molecules: (ABX, AMX, ABC, A2B2, etc. types), spin decoupling. FT-NMR (qualitative idea) and its advantages, Applications of NMR in medical diagnosis.

#### Reference Books

- 1) Organic Spectroscopy – W. Kemp
- 2) Introduction to Organic Spectroscopy – L.K. Pavia, Lampman and Kriz
- 3) Spectrometric Identification of Organic Compounds – R. M. Silverstein, G. C. Bassler and T. C. Morrill
- 4) Organic Spectroscopic Analysis – R.J. Anderson, D.J. Bendelm & P.W. Groundwater

**Unit 2: Emission spectroscopy, Atomic absorption and Atomic Fluorescence spectrometry 12L**

Emission Spectroscopy: FC principle. Mirror-image symmetry. Radiative and radiationless, deactivation. Polarization characteristics of emission. Quenchers and lifetime variations. Fluorescence and Phosphorescence. Atomic emission, Atomic absorption and Atomic fluorescence spectrometry: Instrumentation, Typical application, ICP Atomic Fluorescence Spectroscopy, comparison of Methods: ICP verses AAS.

**CH5271: Organic Chemistry Laboratory-II****- 02 Credit****Extraction of organic compounds from natural sources**

Isolation of caffeine from tea leaves.

Isolation of lycopene from tomatoes.

Isolation of beta-carotene from carrot

Isolation of cinnamaldehyde from cinnamon

Isolation of (+)-limonene from orange skin.

Isolation of rose oil from rose.

**Multi-step synthesis of organic compounds**

Salicylaldehyde → Coumarin-3-carboxylic acid → Coumarin.

Diacetone alcohol → mesityl oxide → dimedone.

Benzoin → Benzil → Benzilic acid.

Skraup synthesis: Preparation of quinoline from aniline.

Fischer-Indole synthesis: Preparation of 2-phenyl indole from phenylhydrazine.

Synthesis of fluorescent dyes.

**Reference Books:**

- 1) Vogel's Text Book of Practical Organic Chemistry – A.R. Tatchell
- 2) Introduction to Organic Laboratory technique – Pavia, Lampman, Kriz & Engel
- 3) Organic Experiments – K.L. Williamson
- 4) General Chemistry Experiments – A.J. Elias
- 5) Comprehensive Practical Organic Chemistry – V.K. Ahluwalia & R Agarwal

**CH5272: Physical Chemistry Practical –I****- 02 Credit**

1. Conductometric titration of a mixture of Hydrochloric acid, potassium chloride & ammonium chloride with silver nitrate and sodium hydroxide.
2. Verification of Onsager equation and thereby to find out the value of  $\lambda_0$  of  $\text{KNO}_3$ .
3. Potentiometric determination of the strength of chloride, bromide & iodide by titration with silver nitrate.
4. Determination of iso – electric pH of gelatin.
5. Kinetic study of hydrolysis of crystal violet in alkali solution and solvent effect with acetone.
6. Determination of solubility curve of three component systems : i) Water – Acetic Acid – Chloroform & ii) Water-Toluene-Acetic Acid.

**CH5273: Term Paper****- 04 Credit****CH5291: Term Paper Viva****- 02 Credit**

## SEMESTER III

### CH6101: Kinetics, Microscopic Dynamics and Fundamentals of Electrochemistry - 04 Credit

#### Unit 1: Kinetics and Microscopic Dynamics:

24 L

Activated processes and Transition state theory, Thermodynamic of the activated state, Statistical approach to rate theory: Hinshelwood, RRK & RRKM models, Single and double sphere model, Primary kinetic isotope effect, Diffusion controlled reactions, Oscillatory reactions, Autocatalysis.

Stochastic approach (Dynamical Laws) to transport properties in condensed phases, Einstein and Langevin models of Brownian motion, Autocorrelation function, Fluctuation-dissipation theorem, Einstein-Smoluchowski model, Diffusion processes coupled with a chemical reaction, Marcus electrons transfer theory, Coupled Flows: Onsager reciprocal relations.

#### Reference Books:

- 1) Chemical Kinetics by K. J. Laidler
- 2) Foundation of Chemical Kinetics by S. W. Benson
- 3) Principles of Chemical Kinetics by J. E. House
- 4) Introduction to Chemical Kinetics by M. R. Wright
- 5) Physical Chemistry: Kinetics by H. Metiu
- 6) Oscillations, Waves, and Chaos in Chemical Kinetics by S. K. Scott
- 7) Chemical Chaos by Stephen K. Scott
- 8) Molecular Driving Forces by K. A. Dill and S. Bromberg
- 9) Physical Chemistry by Berry, Rice and Ross

#### Unit 2: Fundamentals of Electrochemistry

24L

Ionics: Electrochemistry of solutions, Ion-solvent interactions, ion-ion interactions, ionic migration and diffusion. Phenomenological description of transport processes. Thermodynamics of galvanic cells: Equilibrium electrode potentials, IUPAC convention for electrode potentials, Thermodynamics of electrochemical cells and applications.

Electrical Double layer: Theories of Double-Layer structure, diffuse-double-layer theory of Gouy and Chapman, the Stern Model, Adsorption of ions and neutral compounds, Electrocapillary and differential capacitance measurements; Influence of double layer on charge transfer processes. Electrodes: Reference electrodes: polarizable and non-polarizable systems. Types of reference and working electrodes, Electroactive Layers and Modified Electrodes.

Electrode kinetics: Current-potential relationship (derivation of Butler-Volmer and Tafel equations). Adsorption isotherms for intermediates formed by charge transfer (Langmuir adsorption and its limitations, relating bulk concentration to surface coverage), Types of overpotentials: origin and minimization; mechanism of electroorganic reactions; hydrogen evolution and oxygen reduction reactions. transition state theory and Gibbs free energy of activation, bulk electrolysis; Quadratic activation –driving force relation – Marcus theory ; outer and inner sphere reactions.

Electrochemical Instrumentation.

#### Reference Books:

- 1) Modern Electrochemistry – J.O.M. Bockris & A.K. N. Reddy, Vol. 1 & 2A
- 2) Electrochemical Methods: Fundamentals and Applications, A.J. Bard, Larry R. Faulkner.
- 3) Physical Electrochemistry: Fundamentals, Techniques, and Applications, E. Gileadi and Noam Eliaz.

## **CH6102: Reaction Mechanism and Spectroscopic techniques in Inorganic Chemistry - 04 Credit**

### **Unit 1: Inorganic Reaction Mechanism**

**12L**

Types of mechanisms, Substitution reactions of 4 & 6 coordinated complexes, Kinetics and mechanisms, Trans effect, Trans influence, Base catalysis, Anation, Solvent exchange & solvolytic reaction. Broad classes of mechanism of substitution – ‘D’, ‘A’, ‘Ia’ and ‘Id’. Isomerization reaction – mechanism, linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms.

#### **Reference Books:**

- 1) Inorganic Reaction Mechanism – F. Basalo & R.G. Pearson
- 2) Inorganic Reaction Mechanism – R.B. Jordon
- 3) Reaction Mechanism of Metal Complexes – R.W. Hay

### **Unit 2: Inorganic Electron Transfer Reaction**

**12L**

Factors affecting the rates of reactions- effect of temperature, entropy, external pressure, ionic strength and salt effect; The linear free energy relationship (L.F.E.R.) and its use; Electron transfer reactions- the inner sphere and outer sphere mechanism, Outer sphere reaction: Marcus equation for electron transfer, Franck Condon Principle, Ligand effect on outer sphere electron transfer rate, Inner sphere mechanism: effect of bridging ligand, transfer of bridging ligand.

#### **Reference Books:**

- 1) Inorganic Reaction Mechanism – F. Basalo & R.G. Pearson
- 2) Inorganic Reaction Mechanism – R.B. Jordon
- 3) Reaction Mechanism of Metal Complexes – R.W. Hay

### **Unit 3: Mossbauer and Photoelectron Spectroscopy**

**12L**

Mössbauer spectroscopy: principle, experiment, line-width, center shift, effects of nuclear quadrupole on Mossbauer spectra, magnetic interaction; information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mossbauer active nuclei in variety of environments.

Photoelectron spectroscopy: photoexcitation and photoionization, core level (XPS, ESCA) and valence level (UPS) photoelectron spectroscopy, XPS and UPS experiment, chemical shift, detection of atoms in molecules and differentiation of same element in different environments from XPS, information about the nature of molecular orbital from UPS, UPS of simple diatomic molecules. Concept and application of AES, XRF.

NMR spectroscopy: Proton, fluorine and phosphorous NMR of Inorganic compounds

### **Unit 4: EPR Spectroscopy**

**12L**

EPR spectroscopy: Zeeman interaction and energy levels, g factor, dipolar coupling, Hyperfine coupling and A parameter, super-hyperfine coupling. The electronic ground states of d- electron species; epr parameters of d- electron species; spin – orbit coupling and significance of g-tensors; covalence effects; determination of geometry of Cu(II)-complexes, examples of some typical mononuclear and binuclear complexes including biological systems

#### **Reference Books:**

- 1) Electronic Absorption Spectroscopy – D.N. Satyanarayana
- 2) Structural Methods in Chemistry – E.A. V. Ebbsworth, D.W.H. Rankin
- 3) Inorganic electronic structure and spectroscopy – A.B. P. Lever and E.I. Solomon Ed.
- 4) Symmetry and Spectroscopy – K.V. Reddy
- 5) Physical Methods in Chemistry – R.S. Drago

## CH6103: Chemistry of Natural Product and Supramolecular Chemistry - 04 Credit

### Unit 1: Terpenes and Steroids

12L

Isoprene rule; General methods for determining structure; Introduction, synthesis, and biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes. General introduction to sesqui, di- and tri-terpenes. Total synthesis of Longifolene, Juvabione, Asteriscanolide, and Aphidicolin.

Introduction and stereochemistry of steroids, chemistry of cholesterol, Vitamins D-group, bile acids hormones.

### Unit 2: Alkaloids

12 L

Definition, classification, general methods of isolation, structure elucidation, transformation and biosynthesis of alkaloids from terrestrial and marine sources; synthesis of alkaloids (nicotine, ephedrine, atropine, quinine and morphine), chemistry of indole and peptide alkaloids.

### Unit 3: Carbohydrate, Peptide and Proteins

12 L

Basic structure and type of sugars. Protection and deprotection. Various methods of glycoside bond formation (O-glycosylation and C-glycosylation), Deoxy-sugars, amino sugars, glycal sugars and their synthetic aspects. Carbohydrates as chiral pools in organic synthesis. Chemistry of peptide bonds; synthesis of peptides, N-protection, Carboxy protection, activating agents, determination of N-terminus and C-terminus, Edman degradation; solid phase synthesis of peptides, structural features of proteins, forces responsible for holding of secondary structures;  $\alpha$ -helix and  $\beta$ -sheets.

#### Reference Books:

- 1) Organic Chemistry – I. L. Finar (Vol.II)
- 2) Natural Products: Chemistry & Biological Significance - J. Mann, R.S. Davidson et. al.
- 3) Organic Chemistry – I.L. Finar (Vol.II)
- 4) Outlines of Biochemistry – E.E. Corn & P.K. Stumpf
- 5) Organic Chemistry – Claydon
- 6) Carbohydrate Chemistry – S. Khadem
- 7) Biochemistry – Lehninger
- 8) Classics in Organic Synthesis – K.C. Nicolaou (Vol 1, 2 and 3)
- 9) Classics in Total Synthesis: Targets, Strategies, Methods (1<sup>st</sup> Ed.) – K. C. Nicolaou & E. J. Sorensen

### Unit IV: Supramolecular Chemistry

12 L

Concepts and terminology of supramolecular chemistry. Crown ethers: discovery, nomenclature, synthesis, properties and applications. Rotaxane, Catenane and Cryptands: structures and applications. Molecular recognition: definition, examples of molecular recognition utilizing Hydrogen bonding, van der Waal interactions, electrostatic interactions, solvophobic, pi-pi interaction, etc. Cyclodextrins: Structure, property, applications, Supramolecular Gel, Chemical Sensor for neutral molecules, cation and anion, Photophysical properties of Chemosensors, Calculation of binding constant in different methods.

#### Reference Books:

- 1) Supramolecular Chemistry – Beer, Gale & Smith
- 2) Supramolecular Chemistry- Jean-Marie Lehn Supramolecular Chemistry Series- Ed. JeanMari Lehn
- 3) Supramolecular Chemistry: Concepts and Perspectives, J. M. Lehn, VCH, Weinheim, 1995.
- 4) Principles and Methods in Supramolecular Chemistry, H. J. Schneider and A. Yatsimirsky, Wiley.
- 5) Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John Wiley & Sons, Chichester.
- 6) I. P. Beer, P. Gale and D.Smith , Supramolecular Chemistry (Oxford Chemistry Primers).

**CH6171: Inorganic Chemistry Laboratory-II****- 02 Credit**

Resistivity Measurements of Various Semiconductors and Metallic Thin Films  
Measurements of Hall Voltage of a Semiconductor Material by Hall Probe Method and Determination of Carrier Density  
Spectrophotometric estimation of manganese and chromium using  $\lambda_{\max}$  of  $\text{MnO}_4^-$  and  $\text{Cr}_2\text{O}_7^{2-}$   
Colorimetric study of kinetics of the reduction of  $[\text{Co}(\text{NH}_3)_5\text{N}_3]\text{Cl}_2$  by aqueous  $\text{Fe}^{2+}$  ions  
Colorimetric study of kinetics of the aquation of  $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$   
Determination of Stoichiometry of Metal-Ligand Complex by Job's Method of Continuous Variation  
Determination of Stoichiometry of Metal-Ligand Complex by Mole Ratio method  
Determination of Stoichiometry of Metal-Ligand Complex by Slope ratio method  
Determination of Spectrochemical Series for Cu(II) and Ni(II)  
Colorimetric study of kinetics of degradation of toxic organic dye under visible light using semiconductor thin film

**CH6172: Physical Chemistry Laboratory-II****- 02 Credit**

Determination of the rate constants of the alkaline hydrolysis of ethyl acetate at different temperatures and there by calculation of activation parameters.  
Estimation of  $\text{F}^-$  (mg/lit) in tap water by potentiometric measurements using Fluoride sensitive electrode.  
Determination of hydrolysis constant of Aniline hydrochloride / Lysine hydrochloride.  
Determination of CMC of different surfactants (cationic, anionic and neutral) and their effect on the alkaline fading of crystal violet.  
Determination of Stability constant of Pyridine – Iodine charge transfer complex.  
Determination of Molecular weight of polystyrene from viscosity measurements.  
Study of the kinetics of the Iodination of Acetone.

**CH6173: M. Sc. Thesis Part-I (Progress Report)****- 05 Credit****CH6191: Thesis Progress report Seminar and Viva****- 02 Credit**

## SEMESTER IV

### CH6201: Molecular Quantum Mechanics and Statistical Mechanics

- 04 Credit

#### Unit I: Molecular Quantum Mechanics:

24 L

Vector space formulation of quantum mechanics. Schrodinger representation and Wave mechanics, Time evolution of states and observables, Schrodinger picture vs. Heisenberg picture, Ehrenfest's theorem and classical limit.

Variational Principle (and Linear super position principle), Hellmann-Feynmann Theorem, and Hückel model.

Approximation methods for stationary states: Time independent nondegenerate and degenerate perturbation theory, Stark effect, First and second-order degeneracy lifting

Time dependent perturbation theory, transition probability for a constant and Harmonic perturbation, Fermi-Golden rule, Einstein's A and B coefficients, Adiabatic and sudden approximation, Interaction of atoms with the radiation.

Hund's rule, spin-orbit interaction, exchange energy, Mean-field approximations, Hartree and Hartree-Fock models for closed/open shells, Roothan equation, Koopman's theorem, qualitative idea of spin correlation and pair correlation, methods of capturing the correlation effect and introduction to CI method.

#### Reference Books:

- 1) Introduction to Quantum Mechanics by L. Pauling and E. B. Wilson
- 2) Molecular Quantum Mechanics by P. Atkins
- 3) Elementary Quantum Chemistry by F. L. Pilar
- 4) Applied Wave Mechanics by R. M. Golding
- 5) Quantum Mechanics: Concepts and Applications by N. Zettili
- 6) Quantum Mechanics by Claude Cohen-Tannoudji
- 7) Quantum Mechanics in Chemistry by G. C. Schatz and M. A. Ratner
- 8) Physical Chemistry : A Molecular Approach – D.A. McQuarrie and J. D. Simon
- 9) Physical Chemistry: Quantum Chemistry and Spectroscopy by T. Engel and P. Reid
- 10) Quantum Chemistry by D. A. McQuarrie
- 11) Quantum Chemistry by I. N. Levine
- 12) Introduction to Quantum Mechanics in Chemistry by M. A. Ratner and G. C. Schatz
- 13) Modern Quantum Chemistry- A. Szabo and S. N. Ostlund
- 14) Introduction to Computational Chemistry by F. Jensen
- 15) Quantum Chemistry by A. K. Chandra
- 16) Lectures on Chemical Bonding and Quantum Chemistry by S. N. Datta
- 17) Essentials of Computational Chemistry by C. J. Cramer

#### Unit 2: Statistical Mechanics and its applications

24 L

Introduction: scope of the subject, Phase space and distributions in phase space, Ergodic hypothesis, Liouville's theorem, Concept of ensembles with applications to selective systems, Fluctuations & Stability conditions, Ideal gas in the grand canonical ensemble

Classical and Quantum statistics: Boltzmann, Fermi-Dirac and Bose-Einstein statistics and distribution function, Applications on crystals and gases, Basic theory for electrons in a metal, Bose-Einstein condensation, Transport phenomena.

Virial expansion, Real gases, Introductory nonequilibrium statistical physics: Correlations and response, Elements of Monte Carlo molecular dynamics

#### Reference Books:

- 1) Statistical Mechanics – Donald A. McQuarrie
- 2) Fundamentals of Statistical and Thermal Physics by R., Frederick., McGraw-Hill
- 3) Physical Chemistry – Thomas Engel and Philip Reid
- 4) Physical Chemistry – P. W. Atkins
- 5) Thermodynamics, Kinetic theory, and Statistical thermodynamics - F.W. Sears and G.L. Salinger, Narosa

- 6) Statistical Mechanics by K. Huang 2<sup>nd</sup> ed. Wiley, 1987
- 7) Statistical Mechanics by R. K. Pathria, Pergamon Press, 1972.
- 8) The Elements of Classical Thermodynamics for Advanced Students of Physics by A. B. Pippard. University Press

## **CH6202: Chemistry of f-block, Photochemistry, Clusters and Crystallography - 04 Credit**

### **Unit 1: Chemistry of f-block elements**

**12L**

Stable Oxidation states, Lanthanide and Actinide contraction, Differences between 4f and 5f orbitals, Absorption spectra, magnetic properties, Separation, organometallics of lanthanides and actinides, Applications. Spectral properties of Lanthanide and actinide complexes, f-f transitions, f-d transitions and their sensitivity to ligand environment.

Reference Book: Inorganic Chemistry: Cotton & Wilkinson, Chemistry of the Elements: N N Greenwood & A Earnshaw

### **Unit 2: Cluster compounds**

**12L**

Cluster classification, skeletal electron (Elm) counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, higher boron hydrides structures and reactions, equation of balance, Lipscomb topological diagrams, polyhedral skeletal electron pair theory (PSEPT), carboranes, metalloboranes and heteroboranes, metallocarboranes, zintl ions, Chevrel compounds, molybdenum blue, tungsten blue, ruthenium blue, platinum blue, tungsten bronze, ruthenium red. Iso- and hetero-polyoxometalates of V, Mo and W

### **Unit 3: Inorganic Photochemistry**

**12L**

Structure, bonding and excited states of metal complexes; properties of excited states of metal complexes; photophysical and photochemical pathways; electron transfer reactions of metal complexes; photochemistry of polypyridyl and porphyrin complexes; organometallic photochemistry, bioinorganic aspects of inorganic photochemistry; applications of inorganic photochemistry.

### **Unit 4: Crystallography and superconductivity**

**12L**

Unit cell, Bravais lattice, Crystal system & symmetry, Crystal planes, Miller indices, Reciprocal lattice, X-ray diffraction, Laue equations, Bragg's Law, Various X-ray diffraction methods, Debye-Scherrer method, Diffractometer, Systematic absences, Indexing

Meissner effect, Critical temperature, field & current, Type I & Type II superconductors, Vortex state, Persistent current & Flux quantization, Specific heat, Isotope effect, London

### **Reference Books:**

- 1) Elements of Inorganic photochemistry – G.J. Ferrandi
- 2) Supramolecular Photochemistry – V. Balzani & F. Scandola
- 3) Inorganic Chemistry: Principles of Structure and Reactivity- Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi James E. Huheey
- 4) Chemistry of the Elements- N . N . Greenwood and A. Earnshaw
- 5) Concise Inorganic Chemistry- J.D. Lee
- 6) Fundamentals of Crystallography- Edited by C. Giacovazzo
- 7) Nanostructures and Nanomaterials- G. Cao, Y. Wang
- 8) Nanoscale materials in chemistry- Kenneth J Klabunde, Ryan M Richards
- 9) Solid State Physics – A.J. Dekker
- 10) Introduction to Solid State Physics – Charles Kittel



## CH6203: Advanced Methods in Organic Synthesis

- 04 Credit

### Unit 1: Cross-Coupling and Annulation Reactions

12 L

Transition-metal-catalyzed/promoted (Pd, Cu, Ni, Fe) C–C and C–heteroatom coupling reactions and annulation reactions (Heck, Suzuki, Negishi, Stille, Kumada, Hiyama, Glaser, Ullmann, Sonogashira, Buchwald-Hartwig, Tsuji-Trost) and their applications in organic synthesis.

### Unit 2: C–H Bond Activation, Metathesis and Domino/Tandem/Cascade Reactions

12 L

Transition-metal-catalyzed (Ru, Rh, Pd, Cu) C–H bond activation/functionalization reactions and their synthetic utility.

Olefin metathesis, various types of metathesis and application to organic synthesis.

Introduction to domino/tandem/cascade reaction concepts with selected examples.

### Unit 3: Asymmetric Synthesis and Synthesis of Some Bio-active Molecules

24 L

Concise introduction to asymmetric synthesis, discussion on resolution, chiral auxiliaries, chiral ligands, chiral catalysts and chiral organocatalysts with specific examples, Asymmetric synthesis of menthol (Takasago), crixivan (Merck).

Total synthesis of Biotin, Taxol, calicheamicin  $\gamma$ 1, Hirsutene, Tetrodotoxin, Palytoxin, prostaglandins (PG), azidothymidine (AZT), erythromycin, Reserpine, Ibogamine, Fredericamycin A

### Reference Books:

- 1) Modern methods of Organic Synthesis – W. Carruthers
- 2) 2 Advanced Organic Chemistry, A. Cary and R. I. Sundberg, (Part A and B),
- 3) Organic Chemistry, Clayden, N. Greeves, and S. Warren, (Oxford University Press),
- 4) Modern Organic Synthesis-An Introduction, G. S. Zweifel and M. H. Nantz,
- 5) Comprehensive organic synthesis, B. M. Trost and I Fleming, (Pergamon Press),.
- 6) Transition Metals in the Synthesis of Complex Organic Molecules, L.S. Hegedus, , (University Science)
- 7) Organotransition Metal Chemistry: Applications to Organic Synthesis, S. G. Davis, (Pergamon Press),
- 8) Transition Metals in the total synthesis of complex organic molecules, L. S. Hegedus, (University Science)
- 9) Organic Synthesis using transition metals, Roderick Bates, (Wiley).
- 10) Domino Reactions in Organic synthesis, F. Tietze, G. Braschew, K. gericke, (Wiley)

## CH6221: Medicinal Chemistry and Synthesis of Selective Drugs

- 03 Credit

### Unit 1: Drug design and Mechanism

12L

History of medicinal chemistry, general mechanism of drug action on lipids, carbohydrates, proteins and nucleic acids., physiochemical principles and basis of drug design, quantitative description, Drug transport mechanism and absorption processes. Pharmacodynamic and Pharmacokinetic aspects, Prodrugs and Bioactivation, Computer aided drug designing QSAR, Molecular modelling.

Antigen and antibody: antigen, antigenic determinant, immunopotency, structure of antibody, constant and variable regions, Measurement of antigenantibody interaction, ELISA, western blotting.

### Unit 2: Synthesis of common diseases based Drugs

12L

Antimicrobial, anticancer, antidiabetic, antiinflammatory, antitubercular drugs and cardiovascular drugs: Cardiotonic, Antihypertensive, Antirhythmic and Lipotropic drugs and their mechanism of action.

### Unit 3: Synthesis of Selective drugs

12L

Antibiotics and Vitamins: Synthesis of different type of antibiotics, penicillines, tetracyclines, norfloxacin, ofloxacin and levofloxacin, prostaglandins, cephalosporin, progesterone, longifolene, vitamin B-complex, vitamin C etc.

**Reference Books:**

- 1) The Organic Chemistry of Drug Design and Drug Action – R.B. Silverman;
- 2) Medicinal Chemistry – A. Kar;
- 3) Medicinal Chemistry – F.D. King;
- 4) Text Book of Organic Medicinal and Pharmaceutical Chemistry, I. Wilson, Giswald and F. Doerge,
- 5) Medicinal Chemistry, Wiley Interscience, A. Burger, (Vol. I and II),
- 6) Bentley and Driver's Text Book of Pharmaceutical Chemistry revised by L.M. Artherden, (Oxford University Press)

**CH6222: Advanced Inorganic Chemistry****- 03 Credit****Unit 1: Advance Magnetochemistry****12L**

Spin – orbit coupling and magnetic properties of A, E & T terms arising out of different Russell – Saunders states, Comparison of Experimental data with theoretical calculations, anomalous magnetic moments, magnetic properties of binuclear and polynuclear complexes—ferromagnetism and anti-ferromagnetism

**Unit 2: Bio-inspired Coordination Chemistry and Homogeneous Catalysis****12L**

Different types of ligands, their coordination modes, electron transfer in coordination complexes, structure-bonding correlation, application of simple coordination in homogeneous catalysis, catalysis involving noble metals, catalysis using 3d-base metals, advantages/disadvantages of using noble/3d-base metals in catalysis, metal-ligand cooperative approach in homogeneous catalysis, catalytic oxidation reactions, oxygen transfer from peroxo and oxo species, epoxidation reactions; carbene/nitrene transfer reactions, selected annulation reactions, selected examples of catalytic synthesis of organo-heterocycles. Catalyst poisoning.

**Unit 3: Quantitative basis of Crystal Fields****12L**

Crystal Field Theory, Octahedral, tetrahedral, square planar and tetragonally distorted octahedral Crystal Field potential, The effect of  $V_{\text{oct}}$  and  $V_{\text{tet}}$  on the d wavefunctions, the evaluation of  $\Delta$ , Energy level of transition metal ions, Effect of  $V_{\text{oct}}$  on F-term, Quantitative idea of Orgel and Tanabe-Sugano diagram.

**Reference Books:**

- 1) Ligand Field Theory – B.N. Figgis
- 2) Ligand Field Theory – C.J. Ballhausen
- 3) Inorganic Electronic Spectroscopy – A.B.P. Lever
- 4) Magnetochemistry – R.L. Dutta and A. Syamal
- 5) Magnetochemistry – F.E. Mabbs and D.J. Machine
- 6) Organometallic Chemistry – R.C. Mehrotra and A. Singh
- 7) Organometallic Chemistry – R.H. Crabtree
- 8) Organometallic Chemistry – M. Bochmann (Oxford series)

**CH6223:Computational Chemistry and Numerical Analysis****- 03 Credit****Unit 1: Computational Chemistry****24 L**

Number systems: Decimal, hexadecimal, binary, octal, binary arithmetic

Introduction to FORTRAN Programming: Elements of Fortran programming, constants, variables and operators, arithmetic statements, expressions and hierarchy, library functions, relational operators. Input and output statements, format statements, control statements, loop structures, subscripted variables and arrays. DATA statements, Disk I/O.

Application to Numerical problems: Writing, executing and running simple FORTRAN programs: sorting of data, generation of Fibonacci series, sum of terms in the series expansion of  $\sin x$ ,  $\cos x$ ,  $\log x$ ,  $e^x$  etc., evaluation of the polynomial function and its first derivative, matrix representation and matrix algebra, simple applications in chemical problems etc.

**Unit 2: Numerical Analysis****12 L**

Error analysis: Error, accuracy and precision; Truncation and round-off errors; Mean, Standard deviation, Error propagation. Regression Analysis: Linear regression; Curve Fitting Least squares; Interpolation; Newton's Difference Formula; Cubic Splines, Numerical Differentiation and Integration.

**Reference Books:**

- 1) FORTRAN 77 and Numerical Methods, by C. Xavier, New age International (P) Ltd.
- 2) Numerical Recipes in Fortran 77: volume 1 by W. H. Press and B. P. Flannery, S. A. Teukolsky, W. T. Vetterling; Cambridge University Press
- 3) Introduction To Error Analysis: The Study of Uncertainties in Physical Measurements by J. R. Taylor; University Science Books
- 4) Data Reduction and Error Analysis for the Physical Sciences by Philip Bevington and D. Keith Robinson; McGraw Hill Education

**CH6224: Principles and applications of electrochemistry****- 03 Credit****Unit 1: Electrochemical methods****12L**

Controlled-potential & Controlled-Current techniques. Polarography and Voltammetry. Method Involving Forced Convection-Hydrodynamic Methods. Techniques Based on Concepts of Impedance. Bulk Electrolysis Methods. Electrode Reactions with Coupled Homogeneous Chemical Reactions. Spectroelectrochemistry and Electrogenerated Chemiluminescence.

**Unit 2: Electrochemistry of Materials****12L**

Corrosion: Different types of corrosion; influence of environment; Evans diagram, Pourbaix diagram; corrosion rate measurements; Stern Geary equation; polarization and passivation, mixed potential theory and prevention of corrosion. Underpotential deposition of metals and Electrocatalysis

**Unit 3: Electrochemical energy systems****12L**

Available energy options - their advantages and disadvantages. Electrochemical power sources - theoretical background on the basis of thermodynamic and kinetic considerations. Primary & Secondary cells - Batteries for electric vehicles - present status. Fuel cells - classification - chemistry of fuel cells - detailed description of hydrogen/oxygen fuel cells - methanol - molten carbonate solid polymer electrolyte and biochemical fuel cells. Solar energy conversion devices - photoelectrochemical cells - semiconductor electrolyte junctions; photocatalytic modes for fuel conversion process.

**Reference Books :**

- 1) Electrochemical Methods: Fundamentals and Applications, A.J. Bard and Larry R. Faulkner.
- 2) Modern Electrochemistry, J.O.M. Bockris & A.K. N. Reddy – Vol. 2A & 2B
- 3) Analytical Electrochemistry, Joseph Wang
- 4) Fundamentals of electrochemistry, V. S. Bagot'skii
- 5) Physical Electrochemistry: Fundamentals, Techniques, and Applications, E. Gileadi and Noam Eliaz.
- 6) Chemical and Electrochemical Energy systems, R. Narayan and B. Viswanathan.
- 7) Recent Trends in Fuel Cell Science and Technology, S. Basu
- 8) Fuel Cell Fundamentals (English, Hardcover, O'Hayre Ryan

**CH6271: M.Sc Thesis Part-II****- 08 Credit****CH6291: Thesis Seminar & Viva voce****- 04 Credit**