



**UNIVERSITY OF RAJASTHAN**  
**JAIPUR**

**SYLLABUS**

**M.SC. CHEMISTRY**

**Semester Scheme**

<b>I/II Semester Examination</b>	<b>2017-2018</b>
<b>III/IV Semester Examination</b>	<b>2018-2019</b>

**Dy. Registrar**  
**(Academic)**  
**University of Rajasthan**  
**JAIPUR**

# M.Sc. CHEMISTRY

Syllabus 2017-2019

## Credit-based Semester System with continuous assessment.

To acquire a Master degree in Chemistry, a candidate is required to earn minimum of 120 credits with grade E or higher.

Credit registration at least once in all Compulsory Credit Course (CCC) and earning all credits for accumulation of the prescribed minimum credit with grade E or higher grade in all CCC will be binding.

### SCHEME OF EXAMINATION:

- Each Semester shall have continuous assessment which shall include internal assessment in theory and practical by internal examination/seminar/oral examination/viva-voce etc, besides assessment of candidate's regularity and performance in the class.
- A candidate has to pass in the continuous assessment as well as EoSE (End of Semester Examination) paper separately.
- Each EoSE of theory paper shall carry 100 marks and will be of 3 hours duration. Candidate has to attempt five (05) questions in all. All questions carrying equal marks.
- Part 'A' of the theory paper shall contain 10 Short Answer Questions of total 20 marks, based on knowledge, understanding and applications of the topics/texts covered in the whole syllabus. Each question will carry two (02) marks for correct answer.
- Part 'B' of the theory paper will have total four questions of 20 marks each, framed by taking one question from each unit with internal choice. The limit of answer will be five pages.
- Each Laboratory EoSE will be of six hours durations and involve laboratory experiments/exercises, record and viva-voce examination with weightage in ratio of 75:25.
- The Practical examination will be conducted by board of examiners consisting of one internal (to be appointed by the Head of Department) and one external examiner (to be appointed by the University).
- The medium of instruction and examination shall be English only.

### COURSE STRUCTURE

The Credit Courses of the programme have been classified as below:

- CCC: Compulsory Core Course
- ECC: Elective Core Course
- SSC: Self Study Course
- PRJ: Project Work

Dy. Registrar  
(Academic)  
University of Rajasthan  
JAIPUR

**M.Sc. Chemistry I & II Semester (2017-18) III & IV Semester (2018-19)**

**FIRST SEMESTER**

S. No	Subject Code	Course Title	Course Category	Credit	Contact Hours/week					EoSE (hrs)
					L	T	P	Th	P	
1.	CHE 701	Advanced Inorganic Chemistry-I	CCC	4	4	0	0	3	0	
2.	CHE 702	Organic Reaction Mechanism	CCC	4	4	0	0	3	0	
3.	CHE 703	Quantum, Surface and Electrochemistry	CCC	4	4	0	0	3	0	
4.	CHE 711	Chemistry Core Laboratory-1	CCC	6	0	0	9	0	6	
5.	CHE A01	Spectroscopy – I	ECC	4	4	0	0	3	0	
6.	CHE A02	Analytical Techniques	ECC	4	4	0	0	3	0	
7.	CHE A03	Green and Sustainable Chemistry	ECC	4	4	0	0	3	0	
8.	CHE A11	Elective Laboratory-1	ECC	6	0	0	9	0	6	

**SECOND SEMESTER**

S. No	Subject Code	Course Title	Course Category	Credit	Contact Hours/week					EoSE (hrs)
					L	T	P	Th	P	
1.	CHE 801	Advanced Inorganic Chemistry– II	CCC	4	4	0	0	3	0	
2.	CHE 802	Stereochemistry & Organic Reaction Mechanism II	CCC	4	4	0	0	3	0	
3.	CHE 803	Thermodynamics and Chemical Kinetics	CCC	4	4	0	0	3	0	
4.	CHE 811	Chemistry Core Laboratory-2	CCC	6	0	0	9	0	6	
5.	CHE A04	Spectroscopy – II	ECC	4	4	0	0	3	0	
6.	CHE A05	Environmental Chemistry	ECC	4	4	0	0	3	0	
7.	CHE D01	Biomolecules – I	ECC	4	4	0	0	3	0	
8.	CHE A12	Elective Laboratory – 2	ECC	6	0	0	9	0	6	

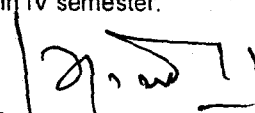
**THIRD SEMESTER**

S. No	Subject Code	Course Title	Course Category	Credit	Contact Hours/week					EoSE (hrs)
					L	T	P	Th	P	
1.	CHE 901	Organotransition Metal Chemistry	CCC	4	4	0	0	3	0	
2.	CHE 902	Organic Synthesis – I	CCC	4	4	0	0	3	0	
3.	CHE 903	Bio-Physical Chemistry	CCC	4	4	0	0	3	0	
4.	CHE 911	Core Laboratory – 3	CCC	6	0	0	9	0	6	
5.		Theory Elective – 1	ECC	4	4	0	0	3	0	
6.		Theory Elective – 2	ECC	4	4	0	0	3	0	
7.		Theory Elective – 3	ECC	4	4	0	0	3	0	
8.		Elective Laboratory-3	ECC	6	0	0	9	0	6	

**FOURTH SEMESTER**

S. No	Subject Code	Course Title	Course Category	Credit	Contact Hours/week					EoSE (hrs)
					L	T	P	Th	P	
1.	CHE X01	Solid States and Nanomaterials	CCC	4	4	0	0	3	0	
2.	CHE X02	Organic Synthesis – II	CCC	4	4	0	0	3	0	
3.	CHE X03	Advanced Physical Chemistry	CCC	4	4	0	0	3	0	
4.		Theory Elective – 1	ECC	4	4	0	0	3	0	
5.		Theory Elective – 2	ECC	4	4	0	0	3	0	
6.		Theory Elective – 3	ECC	4	4	0	0	3	0	
7.		Elective Laboratory – 4	ECC	6	0	0	9	0	6	
8.		Elective Laboratory – 5	ECC	6	0	0	9	0	6	
9.		Project Work*	PRJ	12						

Students will have option of Project work of 12 credits in place of two Elective labs in IV semester.

  
**Dy. Registrar**  
 (Academic)  
 University of Rajasthan  
 JAIPUR

**Elective Core Courses (ECC) groups****A: Integrated / Allied Chemistry****B: Inorganic Chemistry group****C: Physical Chemistry group****D: Organic Chemistry group****E: Pharmaceutical Chemistry group**

S. No.	Course Code	Elective Paper Title	Prerequisite	Semester
1.	CHE A01	Spectroscopy – I		I
2.	CHE A02	Analytical Techniques		I
3.	CHE A03	Green and Sustainable Chemistry		I
4.	CHE A04	Spectroscopy – II		II
5.	CHE A05	Environmental Chemistry		II
6.	CHE B01	Bioinorganic Chemistry	-	III
7.	CHE B02	Supramolecular Chemistry	-	III
8.	CHE B03	Inorganic Polymers	-	III
9.	CHE B04	Advanced Bioinorganic Chemistry	CHE B01	IV
10.	CHE B05	Materials and Industrial Chemistry	-	IV
11.	CHE B06	Photoinorganic Chemistry	-	IV
12.	CHE C01	Advanced Electrochemistry – I	-	III
13.	CHE C02	Advanced Chemical Kinetics – I	-	III
14.	CHE C03	Chemical Analysis	-	III
15.	CHE C04	Advanced Chemical Kinetics – II	CHE C02	IV
16.	CHE C05	Advanced Electrochemistry – II	CHE C01	IV
17.	CHE C06	Advanced Nanoscience and Nanotechnology	-	IV
18.	CHE D01	Biomolecules – I	-	II
19.	CHE D02	Heterocyclic Chemistry – I	-	III
20.	CHE D03	Natural Product – I	-	III
21.	CHE D04	Medicinal Chemistry – I	-	III
22.	CHE D05	Heterocyclic Chemistry – II	CHE D02	IV
23.	CHE D06	Natural Product – II	CHE D03	IV
24.	CHE D07	Medicinal Chemistry – II	CHE D04	IV
25.	CHE E01	Pharmaceutical Chemistry – I		III
26.	CHE E02	Biomolecules II	CHE D01	III
27.	CHE E03	Pharmaceutical Chemistry – II	CHE E01	IV
28.	CHE E04	Advanced Pharmaceutical Chemistry		IV
29.	CHE A11	Elective laboratory – 1	-	I
30.	CHE A12	Elective laboratory – 2	-	II
31.	CHE B11	Elective laboratory – 3	-	III
32.	CHE C11	Elective laboratory – 3	-	III
33.	CHE D11	Elective laboratory – 3	-	III
34.	CHE E11	Elective laboratory – 3	-	III
35.	CHE B12	Elective laboratory – 4/5	-	IV
36.	CHE C12	Elective laboratory – 4/5		IV
37.	CHE D12	Elective laboratory – 4/5	-	IV
38.	CHE E12	Elective laboratory – 4/5	-	IV
39.	CHE A13	Elective laboratory – 5	-	IV
40.	CHE A21	Project Work – PRJ	-	IV

- Department will inform the students about the minimum/maximum number of Elective courses offered to students at the beginning of each semester based on the courses opted by students and availability of faculty.
- Theory elective papers 1-3 to be opted out of one of four elective groups offered, Pharma group students may opt D02/D04 and D05/D07 as third elective in III and IV semester. Elective Laboratory – 3 & 4 will be according to the opted Elective Theory group and student may opt any other laboratory course as Elective Laboratory 5 course.
- The students will have choice to opt project work (12 Credits) or two elective laboratory courses of 6 credits each.

  
**Dy. Registrar**  
(Academic)

University of Rajasthan  
JAIPUR

**CHE 701: ADVANCED INORGANIC CHEMISTRY – I**  
**(Theories of Bonding, Spectroscopic methods and Nuclear Chemistry)**

4 Credit (4 hrs/week)

**UNIT - I**

**Stereochemistry and Bonding in Main Group Compounds:**

Limitations of VSEPR Theory,  $d\pi$ - $p\pi$  bond, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules

**Metal Ligand Bonding:**

Limitation of crystal field theory, molecular orbital theory, and introduction to ligand field theory:  $\sigma$ -bonding in octahedral and tetrahedral complexes,  $\pi$ -bonding and molecular orbital theory.

**UNIT - II**

**Electronic Spectra of Transition Metal Complexes**

Spectroscopic ground states, correlation diagrams, Orgel and Tanabe-Sugano diagrams for transition metal complexes ( $d^1$ - $d^9$  states), calculations of  $Dq$ , Racah parameters ( $B$ ) and nephelauxetic ratio ( $\beta$ ) parameters, charge transfer spectra.

**UNIT - III**

**Optical Rotatory Dispersion (ORD), Circular Dichroism (CD) and Magnetic Properties of Transition Metal Complexes**

Spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical conformation, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

**UNIT – IV**

**Nuclear and Radiochemistry:**

Laws of radioactive decay; Detection of radiations; Geiger-Nuttall rule; GM tubes and their characteristics; Ionization chamber, Proportional counters, Scintillation counters; Solid state detectors; Calibration of counting equipments; Determination of absolute disintegration rates.

**Activation analysis:** Principles; Various methods of activation; Methodology; Advantages, limitations and applications.

**SUGGESTED BOOKS AND REFERENCES**

1. Inorganic Chemistry, Principles of structure and Reactivity, 4<sup>th</sup> Edition; James E. Huheey; Elleu A. Keiter; Richard L. Keiter.
2. Advanced Inorganic Chemistry; F.A. Cotton and G. Wilkinson.
3. Theoretical Inorganic Chemistry; Day and Selbin.
4. Concepts and Models in Inorganic Chemistry; Douglas Mc Daniel.
5. Physical Methods in Inorganic Chemistry; R. S. Drago.
6. Chemistry of the Elements; N.N. Greenwood and A. Earnshaw, Pergamon, 1984.
7. Inorganic Electronic Spectroscopy; A.B.P. Lever, Elsevier, 1968.
8. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty, Pergamon, 1987. Vol. 2.
9. Nuclear and Radiochemistry; G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller; 3<sup>rd</sup> Edn, Wiley; NY, 1981.
10. Essentials of Nuclear Chemistry. H. J. Amikar; 4<sup>th</sup> Eds., New Age International N Delhi, India, 2011.
11. Nuclear and Radiochemistry. Fundamental and Applications, 2 Vols., Jens-Volker Kratz and Karl Heinrich Lieber, 3<sup>rd</sup> Edn. John Wiley & Sons, UK, 2013.

## CHE 702: ORGANIC REACTION MECHANISM

4 Credit (4 hrs/week)

### UNIT- I

#### Reaction Mechanism: Structure and Reactivity

A review of types of mechanisms and reactions, methods of determining reaction mechanism, thermodynamic and kinetic requirements for reaction, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett Principle, Isotope effects. Effects of structure on reactivity, resonance and field effects, steric effects. Quantitative treatment of the effect of structure on reactivity. The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.

**Aromaticity:** Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons. Huckel's rule, energy level of  $\pi$ -molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach, energetic and magnetic concept.

### UNIT - II

#### Aliphatic Nucleophilic Substitution

The  $S_N1$ ,  $S_N2$ , mixed  $S_N1$ - $S_N2$  and SET mechanisms. The  $S_{Ni}$  mechanism. The neighbouring group mechanism - participation by  $\pi$  and  $\sigma$  bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system. Application of NMR spectroscopy in the detection of carbocations. Nucleophilic substitution at the allylic, aliphatic trigonal and a vinylic carbon.

Reactivity - effect of substrate structure, attacking nucleophile, leaving group and reaction medium. Ambident nucleophile, regioselectivity.

#### Aromatic Nucleophilic Substitution

The  $S_{NAr}$ ,  $S_{N1}$ , benzyne and  $S_{RN1}$  mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richte, Sommelet-Hauser and Smiles rearrangements.

### UNIT - III

#### Aliphatic Electrophilic Substitution

Bimolecular mechanisms -  $S_{E2}$  and  $S_{Ei}$ . The  $S_{E1}$  mechanism - electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and solvent polarity on reactivity.

#### Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction.


#### Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity of aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenations (NBS). Oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

### UNIT - IV

#### Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

  
Dy Registrar  
(Academic)  
University of Rajasthan  
JAIPUR

### ➤ Addition to Carbon-Heteroatom Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagent, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Introduction to condensation reactions involving enolates - Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

### Elimination Reactions

The E2, E1 and E1cB mechanisms. Steric orientation of the double bond. Reactivity, effect of substrate structure, the attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic eliminations.

### SUGGESTED BOOKS AND REFERENCES

1. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, McGraw Hill.
2. Mechanism and Structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston).
3. Advanced Organic Chemistry Part-A. F.A. Carey and R.J. Sundberg, 5th Ed. Springer (2007).
4. Physical Organic Chemistry – J. Hine.
5. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes. Longman
6. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers. Oxford University Press (2001)
7. Structure and Mechanism in Organic Chemistry. C.K. Ingold. Cornell University Press.
8. Organic Chemistry. R.T. Morrison and R N. Boyd. Prentice-Hall.
9. Modern Organic Reactions. H O House, Benjamin.
10. Principles of Organic Synthesis. R O C Norman and J.M. Coxon. Blackie Academic & Professional.
11. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.

## CHE 703: QUANTUM, SURFACE AND ELECTROCHEMISTRY

4 Credit (4 hrs//week)

### UNIT - I

**Introduction:** Historical background – Black body Radiation, de-Broglie concept, Heisenberg's Uncertainty Principle. Postulates of Quantum Mechanics, Operators - Linear, Commutator, Hamiltonian, Hermitian and Angular Momentum Operators, Eigen Value and Eigen Functions, Schrodinger's equation, wave function, physical significance of  $\psi^2$ .

**Application of Schrodinger's Equation** to (i) particle in one dimensional box, (ii) particle in three dimensional box, (iii) Simple Harmonic Oscillator, (iv) Rigid Rotor and (v) Hydrogen atom; Radial and angular wave functions, quantum numbers and their significance.

### UNIT-II

**Angular Momentum:** Ordinary angular momentum, Eigen functions and Eigen values of angular momentum, Ladder Operator, Addition of Angular Momentum, Spin, antisymmetry and Pauli's exclusion principle.

**Approximation Method:** The Variation theorem, linear variation principle, perturbation method (First order and nondegenerate). Application of variation method and perturbation method to Helium atom.

**Molecular Orbital Theory:** Basic ideas, criteria of forming MOs, LCAO Concept. Huckel's Molecular Orbital (HMO) theory for conjugated organic systems. Application of HMO to ethylene, allylic, cyclopropanyl, butadiene and cyclobutadiene system.

### UNIT - III

#### Surface Chemistry

**Adsorption:** Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation). Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon)

**Micelles :** Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles. thermodynamics of micellization -phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

### UNIT - IV

#### Electrochemistry

Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern, Graham Devanatham-Mottwatts, Tobin, Bockris, Devanathan models, Over potentials, exchange, current density. derivation of Butler Volmer equation, Tafel plot. Polarography theory, Ilkovic equation; half wave potential and its significance.

#### SUGGESTED BOOKS AND REFERENCES

1. Physical Chemistry by P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Quantum Chemistry, R.K. Prasad, New Age International
5. Micelles, Theoretical and Applied aspects; V. Morat, Plenum Press.
6. Modern Electrochemistry Vol. I & II; J.O.M. Bockris and A.K.N. Reddy Plenum Press New York
7. Physical Chemistry by Puri, Sharma and Pathania Vishal Publications.



**A. Qualitative analysis of mixture consisting of eight cationic / anionic radicals including:**

- a. Interfering anionic radical
- b. Insolubles : oxides, sulphates and halides
- c. Less common metal ions : Tl, W, Mo, Se, Te, V, Th, Ti, Zr, Ce, Li

**B. Purification techniques and Qualitative analysis**

- a. Demonstrations of purification, drying and storage of solvents using various techniques – distillation, steam distillation, vacuum distillation, etc.
- b. Separation of Organic binary mixtures [(one liquid and one solid) or (two solids)] using  $H_2O$ ,  $HCl$ ,  $NaOH$ ,  $NaHCO_3$ , Ether or other reagent and identification of components using chemical tests, IR spectra for functional group identification and preparation of derivatives.

**C. Experiments based on**

**Surface tension**

- i. To study surface tension concentration relationship for solution (Gibbs equation).
- ii. To determine the critical micelle concentration (CMC) of SDS and CTAB by surface tension techniques.

**Adsorption**

- i. Adsorption of Oxalic acid on charcoal
- ii. Adsorption of Acetic acid on charcoal

**Viscosity**

- i. Determination of molecular weight of given polymer (Polyvinyl alcohol, polystyrene, methyl acrylate, etc.) using viscometer
- ii. Experiments based on determination of viscosity of given liquid using Ostwald's viscometer.

## UNIT - I

**Introduction:** Interaction of light with matter, mechanism of absorption and emission of radiation.

**Microwave Spectroscopy:** Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor; Stark effect, nuclear and electron spin interaction and effect of external field applications.

**Vibrational Spectroscopy:** Vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. P.Q.R. branches, breakdown of Oppenheimer approximation; vibrations of polyatomic molecules; selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal ligand vibrations.

**Raman Spectroscopy:** Origin, rotational and vibrational Raman Spectra of diatomic molecules.

## UNIT - II

**Electronic Spectroscopy**

**Atomic Spectroscopy:** Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

**Molecular Spectroscopy:** Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

**Photoelectron Spectroscopy:** Photo-electric effect, ionization process, Koopman's theorem, photoelectron spectra of simple molecules, ESCA, chemical information from ESCA: Auger electron spectroscopy-basic idea.

## UNIT-III

**Magnetic Resonance Spectroscopy**

**Nuclear Magnetic Resonance:** Basic Principle, Spin quantum number, interaction between Spin and a Magnetic Field, Larmor Precession, Relaxation Times; Continuous Wave NMR Spectroscopy, Fourier Transform NMR Spectroscopy; Introduction to Chemical Shift, Spin-spin coupling, Coupling constant. Nuclei other than hydrogen: Nuclei with spin  $\frac{1}{2}$  ( $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{117}\text{Sn}$ ,  $^{119}\text{Sn}$ , etc.), Nuclei with spin greater than  $\frac{1}{2}$  ( $^{14}\text{N}$ ,  $^{11}\text{B}$ ). Quadrupole effects; factors effecting chemical shift in inorganic compounds - geometry, electronegativity, charge, oxidation state, coordination number. Coupling between two or more than two types of NMR active nucleus in a compound (e.g.  $\text{CHFCI}_2$ ,  $\text{HPFCl}$ ,  $\text{HOP(O)FH}$ ,  $\text{HP(O)F}_2$ ,  $\text{BH}_4$ ).

**Electron Spin Resonance:** Basic principles, zero field splitting and Kramer's degeneracy. Isotropic and anisotropic Hyperfine coupling, spin-orbit coupling and significance of g-tensors, factors affecting the 'g' value, its applications to the study of free radicals & fast reactions and application to transition metal complexes; spin Hamiltonian, spin densities and McConnell relationship, applications - spin polarization for atoms and transition metal ions.

## UNIT-IV

**Mossbauer Spectroscopy:** Basic principles, spectral parameters and spectrum display - applications of the technique to the studies of (i) bonding and structures of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  compounds including those

of intermediate spin; (ii)  $\text{Sn}^{2+}$  and  $\text{Sn}^{4+}$  compounds, nature of M-L bond, coordination number, structure; and (iii) detection of oxidation state and in equivalent MB atoms.

**Electron Microscopy:** Basic principles of Electron Microscopy: SEM, TEM, AFM; and their applications in structural analysis.

#### SUGGESTED BOOKS AND REFERENCES

1. Fundamentals of Molecular Spectroscopy, Banewell and McCash
2. Modern Spectroscopy, J.M. Hollas, John Wiley.
3. Applied Electron Spectroscopy for Chemical Analysis D. H. Windawi and F.L. Ho, Wiley Interscience.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F.A. Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Electronic Absorption Spectroscopy and related Techniques, D.N Sathyanarayana
8. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
9. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
10. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
11. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper & Row.
12. NMR Spectroscopy in Inorganic Chemistry, J.A. Iggo, Oxford University Press: Oxford, 1999, pp 1-21; 31-35.
13. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.

## UNIT I

**Statistics – Introduction to Chemometrics**

Limitations of analytical methods, Errors and classification, Determinant, constant and indeterminate, accuracy, precision, minimization of errors, significant figures and computation rules, mean and standard deviation, distribution of random errors, variance and confidence interval, paired *t*-test, least square method, correlation and regression, linear regression.

## UNIT II

**Sampling in analysis**

Definition, theory, basis and techniques of sampling, sampling statistics, sampling and physical state, crushing and grinding, hazards in sampling, techniques of sampling of gases, fluid, solids, and particulates, minimization of variables, transmission and storage of samples, high pressure ashing techniques (HPAT), particulate matter, its separation in gas stream, filtering and gravity separation, analysis of particulate matter like asbestos, mica, dust and aerosols etc.

**Solvent extraction method in analysis**

Principle, classification, theory, instrumentation and applications.

## UNIT III

**Conductometry:**

Important laws, definitions, relations, effect of dilution on conductivity, measurement of conductivity, types of conductometric titrations, its applications and limitations.

**Potentiometry:**

Principle, instrumentation, types of potentiometric titrations and its applications, pH measurements, determination of pH, ion selective electrodes, instrumentation and applications.

## UNIT IV

**Coulometry:**

Introductions, principle, experimental details of coulometry at constant current and constant potential, titrational applications.

**Atomic Absorption Spectroscopy:**

Introduction, principle, Grotrian diagram, instrumentation, applications, detection limit, sensitivity and disadvantages.

**SUGGESTED BOOKS AND REFERENCES**

1. Mendham J., Denney R.C., Barnes J. D., Thomas M.J.K., Vogels' text book of quantitative chemical analysis, 6<sup>th</sup> edition, Prentice Hall, 2000.
2. Skoog Douglas A., Holler F. James, Nieman Timothy A., Principles of instrumental analysis, Saunders College Pub., 1998.
3. Day R. A and A. L. Underwood, Quantitative analysis, Prentice Hall, 1999.
4. Drago R. S., Physical methods in Chemistry, Saunders, 1999.
5. Peters D.G. J. M. Hayes and G. M. Hefige, A brief introduction to Modern chemical analysis, Philadelphia: Saunders, 1976.
6. Ebsworth E.A.V, DWA Rankin and C. Craddock, Structural methods in inorganic chemistry, ELBS.
7. Elan JAD Butter Worth, Photoelectron spectroscopy.
8. Elie E.I., Stereochemistry of carbon compounds, Tata McGraw-Hill

**UNIT – I****Introduction, principle and concepts of Green Chemistry**

Need for green chemistry; Inception and evolution of green chemistry; Twelve principles of green chemistry with their explanations and examples; Designing a green synthesis using these principles; Green chemistry in day to day life.

**UNIT – II****Non-traditional greener alternative approaches**

Different approaches to green synthesis: (a) Uses of green reagents in organic synthesis - Dimethyl carbonate, polymer supported reagents - per acids and chromic acid; (b) Green catalysts, role of catalysis in sustainable development, homogeneous and heterogeneous catalysts; Introduction, advantages and applications of - (i) Nanocatalysts, (ii) Phase transfer catalysts, (iii) Biocatalysts, (iv) Organocatalysts, in organic synthesis.

**UNIT – III****Applications of non-conventional energy sources**

Introduction of microwave induced synthesis: Microwave activation, equipment, time and energy benefits, limitations; Organic transformations under microwaves - Fries rearrangement, Diels-Alder reaction, decarboxylation, saponification of ester, alkylation of reactive methylene compounds; Heterocyclic synthesis -  $\beta$ -Lactams, pyrrole, quinoline.

Introduction of ultrasound assisted green synthesis: Instrumentation, physical aspects, applications in organic transformations.

Electrochemical synthesis: Introduction, synthesis of sebacic acid and adiponitrile.

**UNIT – IV****Environmentally Benign Solutions to Organic Solvents**

Ionic liquids as green solvents: Introduction, properties and types of ionic liquids. Synthetic applications - Diels-Alder reaction, epoxidation and Heck reaction.

Aqueous phase reactions: Enhancement of selectivity, efficiency. Synthetic applications - 1,3-Dipolar Cycloadditions, Carbon-Carbon bond-forming processes and bromination reactions.

Fluorous solvents in green chemistry: Scope, definition and their synthetic applicability.

Role of supercritical carbon dioxide in green chemistry.

Ethyl lactate as a renewable green solvent: Properties and applications.

**SUGGESTED BOOKS AND REFERENCES:**

1. P.A.G. Blackie, Organic synthesis in water, Springer.
2. P.T. Anastas, J.C. Warner, Green Chemistry, theory and practice, Oxford University Press.
3. M. Lancaster, Green Chemistry: An introductory text, Royal Society of Chemistry.
4. V. Polshettiwar, T. Asefa, G. Hutchings, Nanocatalysis: Synthesis and applications, Wiley.
5. M.A. Ryan, M. Finnesand, Introduction to Green Chemistry, American Chemical Society.
6. P.T. Anastas, Handbook of Green Chemistry, John Wiley and Sons.
7. V.K. Ahluwalia, M. Kidwai, New Trends in Green Chemistry, Springer.

**A. Laboratory Estimations**

- i. Estimation of an acid using another standard acid
- ii. Estimation of a base using another standard base
- iii. Estimation of boric acid
- iv. Determination of percentage purity of commercial soda
- v. Determination of percentage of  $\text{CaCO}_3$  in precipitated chalk sample
- vi. Determination of percentage purity of caustic soda
- vii. Determination of alkali content-antacid tablet using HCl

**B. Organic Preparations (single step)**

- i. Preparation of *p*-bromoacetanilide from acetanilide.
- ii. Preparation of *p*-bromoaniline from *p*-bromoacetanilide.
- iii. Preparation of *m*-dinitrobenzene from nitrobenzene.
- iv. Preparation of *m*-nitroaniline from *m*-dinitrobenzene.
- v. Synthesis of adipic acid from cyclohexanol.
- vi. Preparation of 1,1-bis-2-naphthol (BINOL) from  $\beta$ -naphthol.
- vii. Green synthesis of 7-hydroxy-4-methylcoumarin (Pechmann condensation).
- viii. More one step preparations may be added according to requirement of curriculum

**C. Experiments based on -****Phase Equilibrium:**

- i. Determination of congruent composition and temperature of a binary system (e.g., diphenylamine-benzophenone system).
- ii. To construct the phase diagram for three component system (e.g., chloroform-acetic acid water).
- iii. Study of distribution of benzoic acid in benzene and water to show that benzoic acid dimerise in benzene.
- iv. Determine the equilibrium constant for the reaction  $\text{KI} + \text{I}_2 \rightleftharpoons \text{KI}_3$  by distribution method.

**Conductometry**

- v. Verification of Onsager's equation for strong electrolytes (NaCl, HCl,  $\text{KNO}_3$ , KCl) and determination of constant A and B.
- vi. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
- vii. Determination of the strength of strong and weak acids in a given mixture conductometrically.

**CHE 801: ADVANCED INORGANIC CHEMISTRY– II**  
**(Group Theory, Molecular rearrangement processes & Inorganic reaction mechanisms)**  
**4 Credit (4 hrs/week)**

**UNIT-I**

**Symmetry and Group Theory in Chemistry**

Symmetry elements and symmetry operation, definition of group, subgroup, conjugacy relation and classes. Point symmetry group. Schoenflies symbols, representations of groups by matrices (representation for the  $C_{nh}$ ,  $C_{nv}$ , etc, group to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. Derivation of character table for  $C_{2v}$  and  $C_{3v}$  point group. Symmetry aspects of molecular vibrations of  $H_2O$  molecule.

**UNIT-II**

**Molecular Rearrangement Processes**

Electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reductant, chemical activation. Precursor complex formation and rearrangement, nature of bridge ligands, fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

**UNIT-III**

**Inorganic Reaction Mechanism- I**

Basic principles; lability, inertness, stability and instability of coordination compounds; general principles and mechanisms of substitution reactions of tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral complexes; potential energy diagrams, transition states and intermediates, isotope effects, Berry's pseudo rotation mechanism, Swain-Scott equation.

**UNIT-IV**

**Inorganic Reaction Mechanism- II**

Substitution reactions of octahedral complexes; nature of substitution reactions; Theoretical approach to substitution mechanisms; mechanism of substitution reaction of complexes of cobalt; acid hydrolysis and base hydrolysis of Co (III) complexes.

Substitution reactions of square planar complexes; reaction of Pt (II) complexes; trans effect and its applications to synthesis of complexes; theories of trans effect; mechanism of substitution - kinetics of substitution of Pt(II) complexes; factors affecting the reactivity of square planar complexes.

**SUGGESTED BOOKS AND REFERENCES**

1. Inorganic Chemistry, Principles of Structure and Reactivity. 4th Edition, James E. Huheey; Elleu A. Keiter; Richard L. Keiter.
2. Advanced Inorganic Chemistry, F.A. Cotton and G. Wilkinson.
3. Theoretical Inorganic Chemistry. Day and Selbin
4. Concepts and Models in Inorganic Chemistry, Douglas Mc Daniel.
5. Introductory Quantum Chemistry, A.K. Chandra (Tata McGraw Hill)
6. Chemical Applications of Group Theory, F.A. Cotton.

# CHE 802: STEREOCHEMISTRY AND ORGANIC REACTION MECHANISM II

4 Credit (4 hrs/week)

## UNIT I

### Stereochemistry

Optical activity and chirality, elements of symmetry, specification of configuration - molecules with more than one chiral center. D/L, R/S and Threo/Erythro nomenclature.

Prochirality, Homotopic and Heterotopic ligands and faces, Enantiotopic groups and faces, Re/Si Nomenclature. Stereospecific and stereoselective reactions.

Optical activity in the absence of chiral carbon (biphenyls, allenes, spiranes, ansa compounds). Chirality due to helicity. Chirality in the compounds containing N, S and P.

Geometrical isomerism in cyclic and condensed systems, Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity.

Cram's, Prelog's and Horeau's rules. Circular birefringence, CD, ORD, Octant rule, Cotton effect. The axial haloketone rule. Determination of configuration (absolute and relative) and conformation.

## UNIT II

### Organic Photochemistry

Photochemical excitation – interaction of electromagnetic radiation with organic molecules, types of excitations, fate of excited molecules - Jablonskii diagram, intersystem crossing, energy transfer, photosensitization, quenching, quantum yield, Frank-condon principle.

Photochemical reactions of ketones – Norrish type I cleavage, Norrish type II cleavage; photo reductions; Paterno-Buchi reactions; photochemistry of  $\alpha,\beta$ -unsaturated ketones,  $\beta,\gamma$ -unsaturated ketones.

Photochemistry of alkenes: intramolecular reactions of the olefinic bond – cis-trans isomerisation (stilbene), cyclization reactions.

Photochemistry of aromatic compounds: photochemical rearrangement, photostationary state, isomerizations.

## UNIT III

### Pericyclic Reactions

Characteristics and Classification of pericyclic reactions, thermal and photochemical reactions. Molecular orbital symmetry. Woodward-Hoffmann selection rules, Fukui's FMO approach, Woodward-Hoffmann's Conservation of orbital symmetry and correlation diagrams and PMO method.

Electrocyclic reactions: conrotatory and disrotatory motions.  $4n$ ,  $4n+2$   $\pi$  electron and allyl systems. Valence Tautomerism.

Cycloadditions: antarafacial and suprafacial additions,  $4n$  and  $4n+2$   $\pi$  electron systems. Diels-Alder reaction – stereoselectivity (endo, exo), and regioselectivity; normal and inverse electron demand Diels-Alder reactions; asymmetric Diels-Alder reactions; retro-Diels-Alder reactions; 2+2 addition of ketenes. 1,3-dipolar cycloadditions. Cheletropic reactions.

Sigmatropic rearrangements: suprafacial and antarafacial shifts of C-H and C-C bonds. Retention & inversion of configuration. 3,3- and 5,5-sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

## UNIT IV

### Molecular Rearrangements

Mechanistic aspects, nature of the migration, migratory aptitudes, memory effects. A detailed study of the following rearrangements: Benzil-benzilic acid rearrangement, Favorskii rearrangement, Neber rearrangement, Beckmann rearrangement, Hoffmann rearrangement, Curtius rearrangement, Fossen



rearrangement, Wolff rearrangement, Wittig rearrangement, Fritsch-Buttenberg-Wiechell rearrangement, Stevens rearrangement, Chapman rearrangement, Wallach rearrangement. Photochemical rearrangements: rearrangement of 1,4- and 1,5-dienes, di- $\pi$  methane rearrangement. rearrangement of cyclohexadienone (conjugate and cross conjugate), Dienone-Phenol rearrangement.

#### SUGGESTED BOOKS AND REFERENCES

1. E. L. Eliel and Samuel H. Wilen, Stereochemistry of Carbon Compounds, Wiley-Interscience, 1994.
2. D. Nasipuri, Stereochemistry of Organic Compounds, Principles and Applications, New Academic Science Ltd., 2012.
3. P. S. Kalsi, Stereochemistry: Conformation and Mechanism, 7<sup>th</sup> edition, New Age International Publisher Ltd, New Delhi, 2009.
4. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
5. Jerry March, Advanced Organic Chemistry: Reactions Mechanisms and Structure, McGraw Hill, 1977.
6. E. S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston.
7. FA Carey and RJ Sundberg, Advanced Organic Chemistry Part-A, 5<sup>th</sup> Ed. Springer (2007).
8. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, Longman.
9. C.K. Ingold, Structure and Mechanism in Organic Chemistry, Cornell University Press.
10. R.T. Morrison and R.N. Boyd, Organic Chemistry, Prentice-Hall.
11. H.O. House, Benjamin, Modern Organic Reactions.
12. R O C Norman and J.M. Coxon, Principles of Organic Synthesis, Blackie Academic & Professional.
13. S.M. Mukherji and S.P. Singh, Reaction Mechanism in Organic Chemistry, Macmillan.
14. R. B. Woodward and R. Hoffmann, Conservation of Orbital Symmetry, Verlag Chemie: Weinheim (1970).
15. Ian Fleming, Pericyclic Reactions, Oxford Chemistry.
16. S. Sankararaman, Pericyclic Reactions- A Textbook, Wiley-VCH, Weinheim, 2005.
17. Gilbert A and Baggott J., Essentials of Molecular Photochemistry, Blackwell Scientific Publication.
18. Turro N.J., W.A. Benjamin, Molecular Photochemistry.
19. Cox A. and Camp T., Introductory Photochemistry, McGraw Hill.
20. Fleming I., Molecular orbitals and photochemical reactions,
21. Coxon J. and Halton B., Organic Photochemistry. Cambridge University Press.
22. Albright T., Burdet J and Whango M. Orbital interaction in chemistry, Wiley VCH

## CHE 803: THERMODYNAMICS AND CHEMICAL KINETICS

4 Credit (4 hrs/week)

### UNIT-I

#### Classical Thermodynamics

Brief resume of concept of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept and determination of fugacity.

Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient and its determination. Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength.

Application of phase rule to three component systems; second order phase transitions.

### UNIT-II

#### Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properties in terms of partition functions. Application of partition functions.

Heat capacity behavior of solids-chemical equilibria and equilibrium constant in terms of partition functions. Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics distribution Law and application to helium.

### UNIT-III

#### Chemical Kinetics - I

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects : steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Dynamics of chain reactions: (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical reactions (hydrogen-bromine and hydrogen-chlorine).

### UNIT-IV

#### Chemical Kinetics - II

General features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.

Collision theory of reaction rates, Arrhenius equation and the effect of temperature on reaction rate.

Activated complex theory, Modified collision theory (steric effect)

Dynamics of unimolecular reactions Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus (RRKM) theories of unimolecular reactions.

### SUGGESTED BOOKS AND REFERENCES

1. P. W. Atkins, Physical Chemistry, ELBS.
2. K.J. Laidler, Chemical Kinetics, McGraw Hill.
3. J. Rajaraman and J. Kuriacose, Kinetics and Mechanism of Chemical Transformation, Plenum.
4. Samuel Glasstone, Thermodynamics for Chemist, East West Press.
5. R. P. Rastogi and R. R. Mishra, Introduction to Chemical Thermodynamics, Vikash Publication House.
6. Puri, Sharma and Pathania, Principles of Physical Chemistry, Vishal Publication.

**A. Inorganic Preparations:** Following selected inorganic compounds and their studies by IR spectra, Mössbauer, ESR and Magnetic susceptibility measurements. Handling of air and moisture sensitive compounds under vacuum.

- i. Sodium thiosulphate,  $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$
- ii.  $\text{CuCl}_2 \cdot 2\text{DMSO}$
- iii. Tetraamine cupric sulphate  $[\text{Cu}(\text{NH}_3)_4\text{SO}_4] \cdot \text{H}_2\text{O}$
- iv. N,N-bis(salicylaldehyde)ethylenediamine, Salen  $\text{H}_2$ , Co(Salen)
- v. Copper glycine complex – *cis*- and *trans*-bis(glycinato)Copper(II)
- vi. Linkage Isomers: Nitritopentaamminecobalt(III) Chloride,  $[\text{Co}(\text{NH}_3)_5\text{ONO}]\text{Cl}_2$  and Nitropentaamminecobalt(III) Chloride,  $[\text{Co}(\text{NH}_3)_5\text{NO}_2]\text{Cl}_2$
- vii. *Cis*- and *trans*-dichlorobis(ethylenediamine)cobalt(III) chloride,  $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$

**B. Two Step Organic Synthesis**

- |                         |   |                            |   |                           |
|-------------------------|---|----------------------------|---|---------------------------|
| i. Aniline              | → | 2,4,6-Tribromoaniline      | → | 1,3,5-Tribromobenzene     |
| ii. Aniline             | → | Diazoaminobenzene          | → | <i>p</i> -Aminoazobenzene |
| iii. Phthalic anhydride | → | Fluorescein                | → | Eosin                     |
| iv. Phthalic anhydride  | → | Phthalimide                | → | Anthranilic acid          |
| v. Acetanilide          | → | <i>p</i> -Nitroacetanilide | → | <i>p</i> -Nitroaniline    |

The products to be characterized by m.pt / spectral techniques.

**C Experiments based on -**

**Chemical Kinetics**

- i. Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).
- ii. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactant and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
- iii. Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
- iv. Determination of the rate constant for the oxidation of iodide ions by peroxide studying the kinetics as an iodine clock reaction

**Thermodynamics**

- v. Determination of partial molar volume of solute (e.g. KCl) and solvent in a binary mixture.
- vi. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intramolecular interactions (benzoic acid in water and in DMSO-water mixture) and calculate the partial molar heat of solution.

## UNIT I

**Ultraviolet and Visible Spectroscopy**

Various electronic transitions (185-800 nm) Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Woodward-Fieser rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic compounds. Steric effect in biphenyls.

**Infrared Spectroscopy**

Characteristic vibrational frequencies of aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.

## UNIT II

**Mass spectrometry**

Introduction, ion production - EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds common functional groups, molecular ion peak, metastable peak. McLafferty rearrangement. Ring rule, Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

## UNIT III

**Proton Magnetic Resonance Spectroscopy**

Chemically nonequivalent protons, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercapto). Chemical exchange, effect of deuteration. Complex spin-spin interaction between two, three, four and five nuclei (first order spectra). Stereochemistry, hindered rotation. Karplus curve-variation of coupling constant with dihedral angle. Simplification of complex spectra - nuclear magnetic double resonance, NMR shift reagents, solvent effects. Fourier transform technique, nuclear overhauser effect (NOE).

## UNIT IV

**Carbon-13 NMR Spectroscopy**

General consideration, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

**Applications of Spectroscopy** - Problems based on UV, IR, NMR spectroscopy and Mass spectrometry for structural elucidation of organic compounds.

**SUGGESTED BOOKS AND REFERENCES**

1. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Hassler and T.C. Morrill, John Wiley.
2. Fundamentals of Spectroscopy by Banwell and McCash
3. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Lofitus, Wiley.
4. Application of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry D.H. Williams, I. Fleming, Tata McGraw-Hill.
6. Organic Spectroscopy, William Kemp, Macmillan.

## UNIT-I

**Atmospheric Chemistry**

Atmospheric layers, Vertical temperature profile, heat/radiation budget of the earth atmosphere systems. Properties of troposphere, thermodynamic derivation of lapse rate. Temperature inversion. Calculation of Global mean temperature of the atmosphere. Pressure variation in atmosphere and scale height. Biogeochemical cycles of carbon, nitrogen, sulphur, phosphorus oxygen. Residence times. Sources of trace atmospheric constituents: nitrogen oxides, sulphur dioxide and other sulphur compounds, carbon oxides, chlorofluorocarbons and other halogen compounds, methane and other hydrocarbons.

**Tropospheric Photochemistry**

Mechanism of photochemical decomposition of  $\text{NO}_2$  and formation of ozone. Formation of oxygen atoms, hydroxyl, hydroperoxy and organic radicals and hydrogen peroxide. Reactions of hydroxyl radicals with methane and other organic compounds. Reactions of OH radicals with  $\text{SO}_2$  and  $\text{NO}_2$ . Formation of Nitrate radical and its reactions. Photochemical smog, meteorological conditions and chemistry of its formation.

## UNIT-II

**Air Pollution:** Air pollutants and their classifications. Aerosols-sources, size distribution and effect on visibility, climate and health.

**Acid Rain:** Definition, Acid rain precursors and their aqueous and gas phase atmospheric oxidation reactions, damaging effects on aquatic life, plants, buildings and health. Monitoring of  $\text{SO}_2$  and  $\text{NO}_x$ , acid rain control strategies.

**Stratospheric Ozone Depletion:** Mechanism of ozone formation, Mechanism of catalytic ozone depletion, discovery of Antarctic ozone hole and role of chemistry and meteorology, control Strategies.

**Green House Effect :** Terrestrial and solar radiation spectra, major green house gases and their sources and global warming potentials. Climate change and consequences.

**Urban Air Pollution:** Exhaust emissions, damaging effects of carbon monoxide, monitoring of  $\text{CO}$ , control strategies.

## UNIT-III

**Aquatic Chemistry and Water Pollution**

Redox chemistry in natural waters. Dissolved oxygen, biological oxygen demand, chemical oxygen demand, determination of DO, BOD and COD. Aerobic and anaerobic reactions of organic sulphur and nitrogen compounds in water, acid-base chemistry of fresh water and sea water. Aluminium, nitrate and fluoride in water, petrification, sources of water pollution, treatment of waste and sewage, purification of drinking water, techniques of purification and disinfection.

## UNIT-IV

**Environmental Toxicology**

**Toxic Heavy Metals:** Mercury, lead, arsenic and cadmium, causes of toxicity, bioaccumulation, sources of heavy metals, chemical speciation of Hg, Pb, As, and Cd, biochemical and damaging effects.

**Toxic Organic Compounds:** Pesticides, classification, properties and uses of organochlorine and ionospheres pesticides, detection and damaging effects.

**Polychlorinated Biphenyls:** Properties, use and environmental continuation and effects.

**Polynuclear Aromatic Hydrocarbons:** Source, structures and as pollutants.

**Soil and Environmental Disasters:** Soil composition, micro and macronutrients, soil pollution by fertilizers, plastic and metals. Methods of re-mediation of soil. Bhopal gas tragedy, Chernobyl, three mile island, Minamata disease, Seveso (Italy), London smog.

#### **SUGGESTED BOOKS AND REFERENCES**

1. Environmental Chemistry, Colin Baird, W.H. Freeman Co. New York, 1998.
2. Chemistry of Atmospheres. R.P. Wayne, Oxford.
3. Environment Chemistry, A.K. De, Wiley Eastern, 2004.
4. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
5. Introduction to Atmospheric Chemistry, P.V. Hobbs, Cambridge.

**UNIT-I****Carbohydrates**

Structure and biological functions of derivatives of monosaccharides like, Amino sugars Glucosamine and N-Acetylglucosamine; Carboxylic acid sugars- Glucuronic acid and Gluconic acid Sugar phosphates- Adenosine triphosphate (ATP); Sugar alcohols- Maltitol and Lactitol. Structure nomenclature, properties and reactions of oligosaccharides. Structure and biological functions of derivatives of polysaccharides - chondroitin sulphate, heparin and hyaluronan.

**Unit-II****Lipids**

Introduction, nomenclature, classification, and physical properties of fatty acids. Chemical properties of fatty acids - methylation of carboxyl groups, halogen addition reactions, transformation of isolated type fatty acids to conjugated fatty acids and hydrogenation. Nomenclature, classification, structure and function of triacylglycerols, Phospho- and Glycolipids, Definition and classification of lipoproteins. Involvement of lipids in the formation of biological membranes, Introduction of dic lipids, higher alcohols (Waxes and alkoxy lipids) and Cutin.

**UNIT -III****Amino-acids, Peptides and Protein**

Peptide bond, Chemical and enzymatic hydrolysis of proteins to peptides. Synthetic Amino Acids Utilized for Increasing the Biological Value of Food (Food Fortification) - Glutamic Acid, Aspartic Acid, Lysine, Methionine, Phenylalanine, Threonine, Tryptophan. General Remarks Nomenclature, physical properties and sensory properties of Peptides. Structure and use of peptides of interest to food chemists - Glutathione, Carnosine, Anserine and Balenine, Nisin and Lysine Peptides. Secondary structure of proteins- $\alpha$ -helix,  $\beta$ -sheet, forces responsible for holding the secondary structures of proteins.

**UNIT-IV****Transmission of Genetic Information from the Gene to the Protein**

Nucleic acid structure and function - DNA, double helix, DNA replication, Mutation and DNA repair, RNA, types of RNA, transcription, RNA modification, Genetic code, Translation, Transfer RNA, Steps of translation-initiation, elongation and termination, Chromosome organization, Repetitive DNA sequences.

Prokaryotic regulation of gene expression, Eukaryotic control of gene expression, transcriptional regulations.

**BOOKS SUGGESTED:**

1. Principles of Biochemistry, A. I. Lehninger, Worth Publishers.
2. Biochemistry, L.Stryer, W.H.Freeman.
3. Biochemistry, J. David Rawn, Neil Patterson
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry, E.E. Conn and P.K. Stumpf, John Wiley.
6. Food Chemistry, H.D. Belitz et.al., Springer

**A. Laboratory Estimations**

- i. Estimation of ferric ions in ferric alum.
- ii. Estimation of  $\text{Cr}^{3+}$  ions in tannery waste.
- iii. Estimation of available chlorine in bleaching powder.
- iv. Analysis of bauxite with respect to Aluminium (gravimetrically).

**Synthesis of inorganic compounds and their characterization by IR spectroscopy**

- i. Sodium hexanitritocobaltate(III),  $\text{Na}_3[\text{Co}(\text{NO}_2)_6]$
- ii. Sodium tetrathionate  $\text{Na}_2\text{S}_4\text{O}_6$
- iii. Prussian blue,  $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$
- iv. Pentaamminechlorocobalt(III)chloride,  $[\text{CoCl}(\text{NH}_3)_5]\text{Cl}_2$
- v. Hexaamminecobalt(III)chloride,  $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$

**B. Organic Quantitative Analysis**

- i. Estimation of amines using bromate-bromide solution or acetylation method.
- ii. Estimation of phenols using bromate-bromide solution or acetylation method.
- iii. Determination of number of hydroxyl groups in an organic compound by acetylation method.
- iv. Estimation of sugars using Fehling solution method.
- v. Determination of Neutralization Equivalent of given carboxylic acid.
- vi. Determination of Iodine number and saponification value of an oil sample.
- vii Estimation of sulphur by Messenger or Fusion method.

**C. Potentiometry:**

- i. Determination of strengths of halides in a mixture potentiometrically.
- ii. Determination of the valency of Given ions potentiometrically.
- iii. Determination of activity and activity coefficient of the given electrolytes.

**Conductometric Experiments**

- iv. Double displacement & acid base titration
    - a.  $\text{NH}_4\text{Cl} - \text{NaOH} - \text{Mixture of } \text{CH}_3\text{COOH} \text{ \& } \text{HCl}$
    - b.  $\text{NH}_4\text{Cl} - \text{NaOH} - \text{Mixture of } \text{NH}_4\text{Cl} \text{ \& } \text{HCl}$
  - v. Precipitation titration
    - a.  $\text{KCl} - \text{AgNO}_3 - \text{KCl}$
    - b.  $\text{K}_2\text{SO}_4 - \text{BaCl}_2 - \text{K}_2\text{SO}_4$
  - vi. Determination of dissociation constant of weak acids
-



**CHE 901: ORGANOTRANSITION METAL CHEMISTRY**

**4 Credit (4 hrs/week)**

**UNIT-I**

**Synthesis, Properties, Structure and Bonding of:**

(Giving some specific examples)

- (i)  $\eta^1$ - bonded alkyl complexes
- (ii)  $\eta^1$ - carbene and carbyne complexes
- (iii)  $\eta^2$ - alkene and alkyne complexes
- (iv)  $\eta^3$ - allyl complexes
- (v)  $\eta^4$ - dienyl complexes
- (vi)  $\eta^5$ - dienyl complexes

**UNIT-II**

**Metal nitrosyls, cyanides and isocyanides:**

Synthesis, reactions, structure and bonding in metal nitrosyls: nitrosyl complexes, metal cyanides and isocyanides: cyanogens, cyanates and its analogue. Sulfur, selenium and tellurium ion. Diisocyanides, reactions of isocyanide complexes and their uses.

**UNIT-III**

**Synthetic and Catalytic Aspects of Organotransition Metal Chemistry:**

- (i) Transition metal organometallics in organic synthesis
- (ii) Homogenous catalysis by transition metal organometallics
  - (a) Hydrogenation of alkenes
  - (b) Hydrosilylation of alkenes
  - (c) Metathesis of alkenes
  - (d) Oligomerization and polymerization of alkenes and alkynes
  - (e) Hydroformylation of alkenes
  - (f) Acetic acid synthesis and other carbonylation reactions
  - (g) Oxidation of alkenes

**UNIT-IV**

**Catalysis**

- (a) Heterogenous catalysis by organotransition metal compounds
- (b) Fisher-Tropsch synthesis: Methanation reactions, Synthesis of methanol, gasoline production, function of ZSM-5 Zeolite in stabilization of carbene molecule, application of reaction to industry.
- (c) Water gas shift reaction: Role of  $ZnO/Cr_2O_3$  in the reaction, Acetic acid synthesis from water gas shift, Role of Co catalyst.
- (d) Fluxional organometallic compounds: Rate of rearrangement, Simple examples of non rigid molecules in different coordination geometries, classification, future developments.

**SUGGESTED BOOKS AND REFERENCES**

1. J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, Principles and Applications of Organotransition Metal Chemistry, University Science Books, 1987.
2. R.H. Crabtree, The Organometallic Chemistry of Transition Metals, John Willey, 1989.
3. A.J. Pearson, Metalloorganic Chemistry, Wiley, 1985.
4. R. C. Mehrotra and A. Singh, Organometallic Chemistry, New Age International, 1991.
5. J.P. Candlin K. Aayler and D. F. Thomson, Reaction of Transition Metal Complexes, Elsevier
6. M. H. Green, Organometallic Compounds, Vol. II, Methuen, 1968.

## UNIT - I

**Enolate Chemistry**

Formation of enolates, kinetic and thermodynamic control. Reactions of enolate anions with electrophiles: O vs C alkylation. Enolate condensation reactions: Synthetic applications of inter- and intramolecular Aldol condensations, Claisen, Dieckmann, Knoevenagel, Stobbe condensations, Mukaiyama Aldol reaction. Boron enolates. Nozaki-Hiyama-Kishi coupling. Stereoselective enolate reactions: diastereoselection, Zimmermann-Traxler model, Evans model, Noyori open-chain model. Michael addition and related reactions. Baylis-Hillmann reaction, Robinson annulations.  $\alpha$ -Halogenation, Reformatski reaction.

## UNIT - II

**Metal and non-metal mediated oxidation**

Mechanism, selectivity, stereochemistry and applications of Oppenauer oxidations, aromatization, dehydrogenation, cleavage of C=C bond, ozonolysis, epoxidation using peracids, Baeyer-Villiger oxidation. Oxidations using FeCl<sub>3</sub>, DDQ, NBS, lead tetraacetate, selenium dioxide, Ag, Cr and Mn reagents, periodic acid and osmium tetroxide. DMSO-based oxidations. Oxidation of S, Se and N containing compounds.

**Hydroboration:** Introduction, preparation of alkyl- and alkenylboranes. Synthetic transformations: protonolysis, hydrohalogenation, coupling, isomerisation and displacement reactions. Preparation of amines and sulfides *via* hydroboration.

## UNIT - III

**Metal and non-metal mediated reduction**

Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations (using Pd, Pt and Ni catalysts), Clemmensen reduction, Wolff-Kishner reduction, Meerwin-Ponndorf-Verley reduction, dissolving metal reductions, metal hydride reductions (NaBH<sub>4</sub>, LiAlH<sub>4</sub>, DIBAL). Stereoselectivity in hydride transfer reductions, Wilkinson's catalysis. Boranes in reduction. Hydrosilylation. Photoreduction.

## UNIT - IV

**New Synthetic Reactions**

- Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogashira cross coupling, Buchwald-Hartwig amination and Negishi, Kumada coupling reactions.
- C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.
- Multicomponent Reactions: Mannich, Biginelli, Hantzsch, Passerini, Ugi reaction.
- Ring Formation Reactions: Pausan-Khand reaction, Bergman cyclisation, Nazarov cyclisation.
- Click Chemistry: Criteria for Click reaction, Sharpless azide cycloadditions.
- Olefin metathesis: Shrocks, Grubb's 1st and 2nd generation catalyst, Grubb-Hoveyda catalyst. Olefin cross metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM) and applications.
- Other important synthetic reactions: Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction.

**SUGGESTED BOOKS AND REFERENCES**

- Carey A and Sundberg R J. Advanced Organic Chemistry, Part B: Reaction and Synthesis, Springer, 2008.

2. March J, Advanced organic chemistry: Reactions, mechanism and stereochemistry, John Wiley, 2013.
3. Parkanyi C., Theoretical organic chemistry, Elsevier, 1997.
4. Kurti L, Czako B. Strategic applications of named reactions in organic synthesis, Academic Press, 2005.
5. Smith M.B., Organic synthesis, McGraw Hill, 2002.
6. Nicolaou E.J., Classics in total synthesis, Chemie Verlag, 1996.
7. Corey E.J. and Cheng X.M., The logic of chemical synthesis, John Wiley & Sons, 1989.
8. Fieser and Fieser, Reagents for organic synthesis, Wiley, 1967.
9. Wipf P, Handbook of reagents for organic synthesis, John Wiley & Sons, 2005.
10. Greene T, Wuts P.G.M., Protecting group in organic synthesis, John Wiley & Sons, 1989.
11. Carruther W., Modern methods of organic synthesis, Cambridge University Press, 1971.
12. Smith W.A., Bochkor A.F., Caple, R., Organic synthesis: The science behind art, RSC, 1998.

## UNIT I

**Biological Cell and its Constituents:**

Biological Cell, Structure and functions of proteins, DNA and RNA in living system, Helix Coil Transition.

**Cell Membrane and transport of Ions:**

Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport, Nerve conduction, Donnan membrane equilibrium. Active transport mechanisms. Autoanalyzers. Biological Half life, effective half life, Stable isotopes, Radioactive tracer and dilution analysis.

## UNIT II

**Bioenergetics:**

Standard free energy change in biological reactions, Exergonic and endergonic processes, Hydrolysis of ATP, Synthesis of ATP from ADP.

**Biopolymer Interactions:**

Forces involved in biopolymers interactions, Electrostatic charges and molecular expansions, hydrophobic forces, dispersion forces, Multiple Equilibria and various binding process in biological systems. Hydrogen ion titration curve.

## UNIT III

**Statistical Methods in Biopolymer:**

Chain Configuration of macromolecules, statistical distribution end to end dimensions, calculations of average dimension of various chain structure. Polypeptide and protein structure. Introduction to protein folding problems.

**Molecular weights of biopolymers:**

Evaluations of size, shape and extent of hydration of biopolymers by various experiments, determination of molecular weight of biopolymers by light scattering, sedimentation, viscosity and osmotic pressure methods. Bio-degradable polymers.

## UNIT IV

**Biosensors**

Definition, Biosensor system, Bio receptors, surface attachment of biological elements. Electrochemical transducers, placement of biosensors.

**Applications:**

Glucose monitoring, food analysis, DNA biosensors, microbial biosensors, commercialized biosensors, identification of blood glucose (diabetes) and pregnancy test by colorimetric and electrochemical strip.

## SUGGESTED BOOKS AND REFERENCES

1. Satake and Iqbal, Biophysical Chemistry, Discovery Press, 2003.
2. James P Allen, Biophysical Chemistry, Wiley Blackwell Publisher, 2008.
3. Alan Cooper, Biophysical Chemistry, RSC Publication, 2004, ISBN: 978-0-85404-480-1.
4. Upadhyay, Biophysical Chemistry, Himalaya Publishing Publication House, 2014
5. Zhang, Ju and Joseph Wang, Electrochemical Sensors, Biosensors and their Bio-medical Applications, Academic Press, Elsevier, 2008.

## CHE 911: CHEMISTRY CORE LAB – 3

6 Credit (9 hrs/week)

### A. Laboratory Estimations

- i. Spectrophotometric determination of Iron-phenanthroline complex: Job's method of continuous variations.
- ii. Spectrophotometric determination of nickel as nickel dimethyl glyoximate complex.
- iii. Find out the stability constant of metal complexes by Bjerrum's Method.
- iv. Analyse the given sample of Copper Ferrite ( $\text{CuFe}_2\text{O}_4$ ) & determine the amount and percentage of Copper and Iron volumetrically.
- v. Determination of ferrous ( $\text{Fe}^{2+}$ ) and ferric ( $\text{Fe}^{3+}$ ) ions in the given solution.
- vi. Determination of  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  ions in a given solution and estimation of total hardness of water.

### B. Separation & Purification Techniques:

- i. Extraction of organic compound using separating funnel, Soxhlet extraction method
- ii. Purification of organic compounds using Chromatographic methods
- iii. Isolation of caffeine, casein, chlorophyll.

#### Quantitative estimations

- iv. Estimation of number of Functional groups (phenol, amino, methoxy groups) in given organic compounds
- v. Estimation of amino acids and sugar in given samples.
- vi. Estimation of citric acid / vitamin C in citrus juice.

### C. Chemical Analysis

- i. Determine the dissolved oxygen (DO) of the given water sample.
- ii. Determine the biological oxygen demand (BOD) of the given water sample.
- iii. Determine the Chemical Oxygen Demand (COD) of the given water sample
- iv. Determine the Nitrate ( $\text{NO}_3^-$ ) in drinking water sample.
- v. Determine the phenolic substance in the waste water sample
- vi. Determine the amount of free Chlorine in given water sample.
- vii. Determine the amount of Fluoride in given water sample.
- viii. Determine the dissolved  $\text{CO}_2$  in the given water sample.

## CHE B01: BIOINORGANIC CHEMISTRY

4 Credit (4 hrs/week)

### UNIT - I

#### Metals in Life Processes:

Role of metal ions in biological systems; essential and non-essential elements- macro minerals and essential trace elements- synergism and antagonism among essential trace elements; active transport of Na, K, Mg and Ca ions across the biological membrane; elements of bioenergetics with special reference to elements of high energy phosphate bond.

### UNIT - II

#### Electron Carriers and Photosynthesis:

(a) Electron transfer in biology: Structure and functions of electron transfer proteins. Cytochromes and respiratory chain, iron-sulphur proteins rubredoxin and ferridoxins. Synthetic models for  $Fe_4S_4$  cluster only.

(b) Photosynthetic pigments: Photochemistry of chlorophyll molecules, mechanism of photosynthesis, Calvin cycle and Quantum efficiency. Function of photosystem- I and photosystem-II. Cyclic and noncyclic photophosphorylation.

### UNIT - III

#### Transport and Storage of Dioxygen:

Haem proteins and oxygen uptake. Structure and function of haemoglobin, myoglobin. Structural model for dioxygen binding-co-operativity, Perutz mechanism and Bohr effect; non-haem oxygen carriers in some lower animals, haemocyanin and haemerythrin. Model synthetic complexes of iron, cobalt and copper.


### UNIT - IV

#### Nitrogen Fixation:

Nitrogen in biosphere, nitrogen cycle, role of microorganisms in nitrification, nitrogen fixation in soils. Biological nitrogen fixation and its mechanism, nitrogenase, Chemical nitrogen fixation and other nitrogenase model systems.

#### SUGGESTED BOOKS AND REFERENCES

1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill Valley, CA, 1994.
2. H.v.I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, Bioinorganic Chemistry, University Science Books, Mill Valley, CA (USA), 1994.
3. P.S. Kalsi and J.P. Kalsi, Bio-organic, Bio-inorganic and Supramolecular Chemistry, New Age International, 2010
4. G.L. Eichhorn (ed.), Inorganic Biochemistry vol. I and II, Elsevier Scientific Publishing Co., Amsterdam, 1973.
5. Stephen J. Lippard (ed.), Progress in Inorganic Chemistry, Vol 18 and 38, Wiley, 2009

  
Dy. Registrar  
(Academic)  
University of Rajasthan  
JAIPUR

## CHE B02: SUPRAMOLECULAR CHEMISTRY

4 Credit (4 hrs/week)

### UNIT-I

#### Introduction

Definition and development of supramolecular chemistry, classification of supramolecular host-guest compounds. Nature of supramolecular interactions: ion-ion interactions, ion-dipole interactions, dipole-dipole interactions. Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules.

### UNIT-II

#### Molecular Recognition and Crystal Engineering

Receptors, design and synthesis of co receptors and multiple recognition. Hydrogen bonds, strong, weak and very weak H-bonds, utilization of H-bonds to create supramolecular structures, use of H-bonds in crystal engineering and molecular recognition.

### UNIT-III

#### Supramolecular Reactivity and Catalysis

Supramolecular metallocatalysis, biomolecular and abiotic catalysis. Transport processes and carrier design, cation carriers, anion carriers, coupled transport processes.

### UNIT-IV

#### Devices and Chemistry

Supramolecular devices, supramolecular photochemistry, molecular and supramolecular photonic devices, photosensitive molecular receptors. Supramolecular chemistry of Fullerene, Fullerene as guests, Fullerene as hosts, Fullerene as superconducting intercalation compounds.

### SUGGESTED BOOKS AND REFERENCES

1. J.M. Lehn, Supramolecular Chemistry – Concept and Perspectives, VCH, 2006.
2. J.W. Steed and J.L. Atwood, Supramolecular Chemistry, John Wiley & Sons. Inc., 2009.
3. Bio-organic, Bio-inorganic and Supramolecular Chemistry, P.S. Kalsi and J.P. Kalsi, New Age International, 2010.

**UNIT-I****Basic Concepts**

Classification by connectivity, and classification by dimensionality, metal/backbone classification of metal-containing polymers, linear inorganic polymer.

**Unit-II****Synthesis and Characterization**

Step-growth synthesis, chain polymerization, ring-opening polymerization, reductive coupling and other redox polymerization reactions, Inorganic polymer characterization: average molecular masses, and characterizing methods using Gel permeation chromatography and viscosity, degree of polymerization

**Unit-III****Applications**

Polysiloxane and polyphosphazene elastomers, inorganic medical polymers: polysiloxanes and polyphosphazene as bio polymers, Inorganic polymer conductivity: main group inorganic polymers, metal-containing polymers, Luminescent inorganic polymers: Ruthenium polymers for solar energy conversion.

**Unit-IV****Polymetalloenes**

Introduction, Polymetalloenes with short spacers obtained by condensation routes, ring-opening polymerization (ROP) of strained Metalloenophanes, thermal ROP of silicon-bridged [1]Ferrocenophanes, thermal ROP of other strained metalloenophanes, transition metal catalyzed ROP of strained metalloenophanes.

**SUGGESTED BOOKS AND REFERENCES**

1. Ronald D. Archer, Inorganic and Organometallic Polymers, Wiley-VCH
2. J.E. Huheey, Inorganic Chemistry, Harper Row.
3. M.F. Lappert and G.J. Leigh, Developments in Inorganic Polymer Chemistry, ACS Publications, 1963.
4. N.H. Ray, Inorganic Polymers, Academic Press, NY, 1979.
5. F.W. Billmeyer Jr., Textbook of Polymer Science, Wiley, NY, 1977.
6. H.R. Alcock and F.W. Lambe, Contemporary Polymer Chemistry, Prentice Hall
7. I. Manners, Synthetic Metal-Containing Polymers, Wiley-VCH, Weinheim, 2004.
8. A. S. Abd-El-Aziz, I. Manners Eds., Frontiers in Transition Metal-Containing Polymers, Wiley-Interscience, 2007.



## CHE C01: ADVANCED ELECTROCHEMISTRY- I

4 Credit (4 hrs/week)

### UNIT-I

#### Fuel Cells

Electrochemical Energy Generators (Fuel Cells): Hydrogen oxygen cells. Hydrogen Air Cell, Hydrocarbon air cell, alkaline fuel cell, Phosphoric acid fuel cell, Direct NaOH fuel cells, applications of fuel cells.

#### Electro-chemical Energy Storage

Properties of Electrochemical energy storages: measure of battery performance, Charging and discharging of batteries, Storage density, Energy density.

Classical Batteries: (i) Lead Acid (ii) Nickel-Cadmium (iii) Zinc – Manganese dioxide. Modern Batteries: (i) Zinc- Air (ii) Nickel- Metal hydride (iii) Lithium Battery. Future electricity stores: Storage in (i) Hydrogen (ii) alkali metals (iii) Non-aqueous solutions

### UNIT-II

#### Corrosion and Passivity

Electrochemical mechanism of corrosion of metals, thermodynamics and stability of metals, potential - pH (or Pourbaix) Diaphragms, uses and abuses, corrosion current and corrosion potential - Evans diagrams.

Measurement of corrosion rate; weight loss method and Electrochemical method. Inhibition of Corrosion (i) by addition of substrates to the electrolyte environment (ii) By charging corroding method from external source, anodic protection, organic inhibitors. The Fuller theory, Green inhibitors.

**Passivation** : Structure of passivation films, mechanism of passivation, spontaneous passivation, nature's method for stabilizing surfaces.

### UNIT-III

#### Bio-electrochemistry and Bioelectrocatalysis

Membrane potential, simplistic and modern theory, Electrical conductance in biological organisms, electrochemical mechanism of nervous systems, enzymes as electrodes, Biosensors, Bio-electrocatalysis. Enzymes as biological catalysts, immobilization, methods of immobilization.

### UNIT-IV

#### Kinetics of Electrode Process

Essentials of electrode reaction, significance of current density and overpotential in electrode processes, Standard rate constant ( $k^0$ ) and Electron Transfer coefficient ( $\alpha$ ) and its significance, exchange current density. Criteria of irreversibility information from irreversible wave. Koutecky's method, Meits Israel and Gelling's method for determining kinetic parameters for quasireversible and irreversible waves.

#### SUGGESTED BOOKS AND REFERENCES

1. John O'M. Bockris and Amulya K.N. Reddy, Modern Electrochemistry, Volume 2A & 2B, Springer, 2000.
2. Brett CMA and Brett AMO. Electrochemistry. Principle and Applications, Oxford Press, 2005.
3. Joseph Wang, Analytical Electrochemistry, Wiley-VCH Publication, 1985.
4. Zhang, Ju and Joseph Wang, Electrochemical Sensors, Biosensors and their Bio-medical Applications, Academic Press, Elsevier, 2008.
5. A.J. Fry and W.E. Britton, Topics in Organic Electrochemistry, Plenum publishing press, New York, 1980.
6. M. M. Baizer and H. Lund, Organic Electrochemistry, Marcel Dekker, New York, 1988.

## UNIT I

**Kinetics of Atmospheric Reactions**

Physical structure of atmosphere. Chemical composition of atmosphere, Kinetics and mechanism of  $\text{NO}_x$ ,  $\text{ClO}_x$  cycles and  $\text{H}_2 + \text{O}_2$  reaction. Mechanism of general methane oxidation. Kinetics and mechanism of low temperature oxidation of methane.

## UNIT - II

**Radiation Chemistry**

Radiation chemistry and Photochemistry. Radiation chemistry of water and aqueous solutions. Hydrogen atom and hydroxyl radical-oxidizing and reducing conditions. Kinetics and mechanism of photochemical and photosensitized reactions (one example in each case). Stern-Volmer equation and its application. Hole-concept in the presence of semi-conductor photo-catalysts. Kinetics of exchange reactions (mathematical analysis).

## UNIT - III

**Dynamics of Gas-Surface Reactions**

Adsorption/desorption, kinetics and transition state theory, Dissociative adsorption and precursor state. Mechanism of Langmuir's adsorption of the oxidation of carbon monoxide to carbon dioxide. True and apparent activation energies. Industrial importance of heterogeneous catalysis.

**Transition State:**

A brief aspect of statistical mechanics and transition state theory, application in calculation of the second order rate constant for reactions with collision for (i) atom + atom (2) atom + molecule (3) molecule (for both linear and non-linear molecules) + molecule reactions. Solvent effects and thermodynamic formulations. Adiabatic electron transfer reactions. energy surfaces.

## UNIT - IV

**Enzymes and Inhibitors**

Enzyme catalyzed models of 1:2 type enzyme-substrate systems. Kinetics of one enzyme-Two substrate systems and their experimental characteristics. Enzyme inhibitors and their experimental characteristics. Kinetics of enzyme inhibited reactions.

**Micelles Catalysis and Inhibition**

(a) Micelles and their classification, Kinetics and mechanism of micelle catalyzed reactions (first and second order). Various type of micelle catalyzed reactions. Micelle inhibited reactions.

(b) Kinetics and Mechanism of Substitution Reaction: Classification of ligand substitution mechanism, anation and base catalysed Kinetics of anation reactions. Aquation and acid catalyzed Kinetics of aquation reactions (octahedral complexes).

**SUGGESTED BOOKS AND REFERENCES**

1. Henry Taube, S Lippard (Ed.), Progress in Inorganic Chemistry, Vol 30, John Wiley & Sons, NY, 1983.
2. R. Lumry and R.W. Raymond, Electron transfer reaction, Inter-Science Publication, 1997.
3. N.L. Bender, Mechanism of homogeneous Catalysis from protein to protein, Wiley, 1971.
4. A.G. Sykes, Kinetics of Inorganic reactions, Pergamon Press, 1966.
5. S.W. Benson, Jacob Kleinberg, R. Kent Murmana, R.T.M. Fraser, John Bauman, Mechanism of Inorganic Reactions, Academic Press, 1965.
6. H. Taube, Electron transfer reactions in solution, Academic Press, London, 1970.

## CHE C03: CHEMICAL ANALYSIS

4 Credit (4 hrs/week)

### UNIT-I

#### Water Analysis

Sources of water pollution domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis-parameter for analysis color, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. (Measurement of DO, BOD and COD). Pesticides as water pollutants and analysis. Water pollution laws and standards.

### UNIT-II

#### Food Analysis

Moisture, ash, crude protein, fat, crude fiber, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample: HPLC, Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

### UNIT-III

#### Soil and Fuel Analysis

(a) Analysis of soil, moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

(b) Fuel analysis: liquid and gas. Ultimate and proximate analysis, heating values-grading of coal. Liquid fuels flash point, aniline point, octane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.

### UNIT-IV

#### Body Fluids and Drug Analysis

Composition of blood collection and preservation of samples. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid albumin, globulins acid and alkaline phosphatases, Immunoassay: Principle of radio immunoassay (RIA) and applications. The blood gas analysis trace elements in the body.

Narcotics and dangerous drugs classification of drugs. Screening by gas and thin layer chromatography and spectrophotometric measurements.

#### SUGGESTED BOOKS AND REFERENCES

1. G.D. Christian, P.K. Dasgupta, K.A. Schug, Analytical Chemistry, Wiley, 7<sup>th</sup> edn., 2013.
2. D.A. Skoog, D.M. West and F.J. Hooler, S.R. Crouch, Fundamentals of Analytical Chemistry, 9<sup>th</sup> edn., 2014.
3. J.H. Kennedy, Analytical Chemistry – Principles, Saunders College Publishing, New York, 2<sup>nd</sup> edn., 1990.
4. L.G. Hargis, Analytical Chemistry - Principles and Techniques, Prentice Hall, 1988.
5. R.A. Day, Jr. and A.L. Underwood, Quantitative Analysis, 6<sup>th</sup> edn., Prentice Hall, 1991.
6. S.M. Khopkar, Environmental Solution, Wiley Eastern.
7. S.M. Khopkar, Basic Concepts of analysis Chemistry, New Age International, 1998.
8. Alka L. Gupta, Analytical Chemistry, Pragati Publication, 2014.
9. D.C Das, Analytical Chemistry, Prentice Hall India Learning Private Limited, 2010.

## UNIT-I

**Nomenclature of Heterocycles**

Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused, spiro and bridged heterocycles.

**Aromatic Heterocycles**

General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in  $^1\text{H}$  NMR-spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations). Heteroaromatic reactivity.

## UNIT-II

**Non-aromatic Heterocycles**

Strain - bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interactions. Stereo-electronic effects; anomeric and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic electrophilic interactions.

## UNIT - III

**Small Ring Heterocycles**

**Three-membered and Four-membered Heterocycles:** Synthesis and reactions of aziridines, oxiranes, thiiranes, oxaziridines, azetidines, oxetanes, thietanes and azetidinones.

## UNIT-IV

**Five-membered Heterocycles with Two Heteroatoms**

Synthesis and reactions of 1,2- & 1,3-diazoles, oxazoles, thiazoles and azaphospholes.

**Benzo-fused five-membered Heterocycles**

Synthesis, reactions and medicinal applications of benzopyrroles, benzofurans, benzothiophenes and benzimidazoles.

**SUGGESTED BOOKS AND REFERENCES**

1. R.R. Gupta, M. Kumar and V. Gupta. Heterocyclic Chemistry Vol. 1 & 2. Springer India, 1998 & 1999.
2. T Eicher and S. Hauptmann, The Chemistry of Heterocycles, Wiley-VCH, 2003
3. J.A. Joule, K. Mills and G.F Smith, Heterocyclic Chemistry, Chapman and Hall, 1995
4. T.L. Gilchrist, Heterocyclic Chemistry, Longman Scientific & Technical, 1992.
5. G.R. Newkome and W.W. Paudler, Contemporary Heterocyclic Chemistry, Wiley-Inter Science, 1982.
6. R.M. Acheson, An Introduction to the Heterocyclic Compounds, John Wiley, 1977.
7. A.R. Katritzky, C.W. Rees and E.F.V. Scriven (Eds.), Comprehensive Heterocyclic Chemistry II, ISBN: 9780080965185. Elsevier, 1996.

## UNIT- I

**Terpenoids and Carotenoids**

Introduction, occurrence, nomenclature, general methods of structure determination, isoprene rule, stereochemistry and synthesis of following representative molecules: Citral, Geraniol,  $\alpha$ -Terpineol, Menthol, Farnesol, Zingiberene, Phytol, and Abietic acid. Biosynthesis of Terpenoids. General methods of structure determination of  $\beta$ -Carotene and Lycopene.

## UNIT-II

**Alkaloids**

Introduction, occurrence, nomenclature, classification based on structure, isolation, general methods of structure elucidation of alkaloids, stereochemistry and synthesis of the following: Narcotine, Quinine, Reserpine and Morphine.

## UNIT - III

**Steroids**

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrogen and Progesterone. Biosynthesis of cholesterol.

**Plant Hormones**

Introduction, occurrence, isolation and physiological effects of Auxins, Gibberellins (Synthesis of  $GA_3$ ), Cytokinins and Abscisic acid.

**Nutraceuticals and Natural Products**

Occurrence, isolation, biological function and structure elucidation (by spectroscopic methods) of Curcumin, Silymarin, 5-hydroxytryptophan, Chlorogenic acid and Vinpocetine.

## UNIT-IV

**Natural Pigments**

Occurrence, nomenclature and general methods of structure determination. Isolation, structure determination and synthesis of Luteolin, Quercetin, Luteolin, Diadzein, Genistein, and Cyanidin chloride.

Porphyryns: Structure, reactions and synthesis of haemoglobin, chlorophyll, chlorins, bacteriochlorins and purpurin anhydride. Photosensitizers in Photodynamic Therapy.

**SUGGESTED BOOKS AND REFERENCES**

1. J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Natural Products, Chemistry and Biological Significance, Prentice Hall, 1994.
2. I. L. Finar, Organic Chemistry: Vol. 2, ELBS, Longman, 1996.
3. M. Norgradi, Stereoselective Synthesis: A Practical Approach, Wiley-VCH, 1994.
4. S V. Bhat, B.A. Nagasampagi and M. Sivakumar, Chemistry of Natural Products, Narosa Publishing House, 2015.
5. Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Harwood Academic Publishers, 1999.
6. B.A. Bohm, Introduction to Flavonoids, Harwood Academic Publishers, 1998.
7. Ata-ur-Rahman and M.L. Choudhary, New Trends in Natural Products Chemistry, Harwood Academic Publishers, 1998.

## UNIT-I

**Drug Design**

Development of new drugs, procedures followed in drug design, concepts of prodrugs and soft drugs, structure-activity relationship (SAR and QSAR). Factors affecting bioactivity –resonance, inductive effect, isosterism, bio-isosterism, spatial consideration. Theories of drug activity. Elementary treatment of drug receptor interactions.

## UNIT-II

**Pharmacodynamics** : Definition, Receptors and specificity, agonists and antagonists, Site(s) of drug action, Mechanism of Drug action: therapeutic and side effects, elementary treatment of enzyme stimulation, enzyme inhibition, membrane active drugs, Drug metabolism, xenobiotics, biotransformation significance of drug metabolism in medicinal chemistry.

**Pharmacokinetics** : Introduction to drug absorption, disposition and elimination using pharmacokinetics, Clinical Pharmacokinetics: bioavailability, volume of distribution, clearance, elimination, Design and optimization of dosage regimen, Therapeutic drug monitoring, importance of pharmacokinetics and pharmacodynamics in drug development process.

## UNIT-III

**Posology** : Definition, dose-response relationship, potency and effective dose 50 (ED 50), minimal effective concentration, efficacy: time-response graph, onset, duration and termination of action.

**Drug Toxicity and Poisoning** : Types of therapeutic drug toxicity, Mechanism of Toxicity, Dose response complexities. Therapeutic Index, Lethal Dose 50 (LD 50), Adverse drug effects, Principles of treatment of poisoning, Mechanism of Detoxification and testing.

## UNIT-IV

**Bio-statistics** : Introduction its role and use, Collection, Organization: Graphics and pictorial representation of data. Sampling: Random and non random sampling methods, standard deviation and coefficient of variation. Probability, student t-test, F-Test, chi square test, correlation and regression.

**SUGGESTED BOOKS AND REFERENCES**

1. J. Stringer, Basic Concepts in Pharmacology, 3<sup>rd</sup> edn., McGraw-Hill Professional, 2005.
2. B. Katzung, Basic and clinical pharmacology, 11<sup>th</sup> edn., McGraw-Hill medical, 2009.
3. Goodman & Gilman, Pharmacological basis of Therapeutics, McGraw-Hill, 2005.
4. A. Burger & M.E. Wolff (Ed.), Medicinal Chemistry and Drug Discovery, Vol-1, John Wiley, 1994.
5. S.S. Pandeya & J.R Dimmock, Introduction to drug design, New Age International, 2000.
6. D. Lednicher, Strategies for organic drug Synthesis and Design, John Wiley, 1998.
7. Graham & Patrick, Introduction to medicinal Chemistry, 3<sup>rd</sup>edn., OUP, 2005.
8. Bernard Rosner, Fundamental of Biostatistics, 8<sup>th</sup> edn. CENGAGE Learning Custom Publisher, 2016.
9. Skoog & West, Fundamentals of analytical chemistry. CENGAGE, 2013.
10. J. Susan Milton, Statistical methods in biological and health sciences, Tata McGraw-Hill Int. Edition, 1984.
11. J. Susan Milton, Introduction to statistics. Tata McGraw-Hill Int. Edition, 1996.
12. B.K. Mahajan, Methods in Biostatistics. JayPee Brothers, New Delhi, 2002.

# CHE E01: PHARMACEUTICAL CHEMISTRY I

4 Credit (4 hrs/week)

## UNIT- I

### Chemistry of acids and bases

Dissociation of weak acids and bases, Hydrolysis of salts, Amphiprotic salts, Buffer solutions, Buffer capacity, Biological buffers, Ionization of drugs, pKa values of drug molecules, pH indicators .

### Partition coefficient and biopharmacy

Experimental measurement of partition coefficient , Drug absorption, distribution and bioavailability , Passive diffusion, The pH partition hypothesis, Active transport mechanisms, The action of local anaesthetics, Excretion and reabsorption of drugs.

## UNIT- II

### Drug metabolism

Metabolic pathways, Cytochromes P450, Enzyme induction and inhibition, Drug conjugation reactions (Phase 2) Glucuronic acid conjugation. Sulfate conjugation, Amino acid conjugation, Metabolic pathways for common drugs Amfetamines, Barbiturates, Phenothiazines, Sulfonamides, Cocaine, Phenmetrazine, Ephedrine and caffeine, Factors affecting drug metabolism.

## UNIT III

### Stability of drugs and medicines

Oxidation, Stability of free radicals, Prevention of oxidative deterioration, Autoxidation of fats and oils, Ageing, Hydrolysis. Examples of drugs susceptible to hydrolysis, Other mechanisms of degradation.

## UNIT IV

### Kinetics of drug stability

Rate, order and molecularity, Rate equations and first-order reactions, Half-life, Shelf-life, Second-order reactions, Zero-order reactions, Reaction rates and temperature .

## BOOKS AND REFERENCES

1. Essentials of Pharmaceutical Chemistry (third edition) by Donald Cairns, Pharmaceutical Press
2. Organic Medicinal and Pharmaceutical Chemistry, John M. Beale, Jr., John H. Block, Wolters Kluwer
3. Ansel's Pharmaceutical Dosage Forms and Drug Delivery Systems, Loyd V Allen. Wolters Kluwer
4. Drug delivery: principles and applications, Binghe Wang, Teruna Siahaan, Richard soltero, John Wiley & Sons

**UNIT-I**

**Fuel Molecule Metabolism**

Glycogenesis and glycogenolysis. Aerobic Respiration, glycolysis and regulation of glycolysis, citric acid cycle, regulation of the citric acid cycle, Electron transport chain Oxidative Phosphorylation, Regulation of Oxidative Phosphorylation, oxidative stress, anaerobic pathways, Lactic acid fermentation, pentose phosphate pathway.

**UNIT-II**

**Enzymes**

General Remarks, Isolation and Nomenclature of enzymes Enzyme structure and function, Factors that affects enzyme function- enzyme kinetics, Michaelis–Menten kinetics, Cooperativity, Control of enzyme activity- feedback regulation, enzyme inhibition, covalent modification. Enzyme Cofactors Theory of Enzyme Catalysis and Enzymatic Analysis.

**UNIT-III**

**Marine Biomolecules and Application**

Introduction and history of marine biomolecules, Discovery and development of marine pharmaceuticals, Isolation and screening of marine biomolecules, Occurrence, Structure and function of furanone, kainic acid, tyrian purple, ziconotide and dolastatin,

**UNIT-IV**

**Fungal Biomolecules and Biomolecules of Mushrooms**

Fungi as cell factories, Fungal Biofilms: an overview, Fungal biomolecules for food industry. Bioactive biomolecules of mushrooms: food function and medicinal effect of mushroom fungi. Biomolecules and nanotechnology.

**BOOKS AND REFERENCES**

1. [www.mhpracticeplus.com/BBFLS\\_MCAT/mca88351\\_V1](http://www.mhpracticeplus.com/BBFLS_MCAT/mca88351_V1)
2. Biomolecules and Nanotechnology, David S. Goodsell, American Scientist
3. Food Chemistry, H.D. Belitz et al., Springer
4. Fungal Biomolecules: Sources, Applications and Recent Developments, V.K. Gupta et al. Wiley-Blackwell
5. <http://booksite.elsevier.com/9780120885305/casestudies/02-Ch27-P088530web.pdf>
6. Bioactive biomolecules of mushrooms: Food function and medicinal effect of mushroom fungi, Takashi Mizuno, Food Reviews International Volume 11, 1995



## CHE B11: CHEMISTRY ELECTIVE LAB-3

### Inorganic group

- 1. Chromatographic separation** and identification by paper chromatography and determination of R<sub>f</sub> values:
  - Cadmium and Copper.
  - Zinc and Manganese.
  - Arsenic, Antimony and Tin.
  - Lithium, Sodium and Potassium.
  - Fe<sup>3+</sup>, Al<sup>3+</sup> and Cr<sup>3+</sup>
  - Ca<sup>2+</sup>, Sr<sup>2+</sup> and Ba<sup>2+</sup>
  - Ni<sup>2+</sup>, Co<sup>2+</sup>, Mn<sup>2+</sup> and Zn<sup>2+</sup>
  - Cu<sup>2+</sup>, Fe<sup>3+</sup>, Ni<sup>2+</sup> and Ti<sup>4+</sup>
- 2. Cerimetric titration**
  - Standardization of ceric sulphate solution using ferrous ammonium sulphate as intermediate solution
  - Determination of the percentage of H<sub>2</sub>C<sub>2</sub>O<sub>2</sub> in oxalic acid crystals.
  - Determination of percentage purity of a sample of sodium nitrite.
- 3. Estimations**
  - Estimation of H<sub>2</sub>O<sub>2</sub> by iodometric method.
  - Estimation of Zinc involving Potassium ferrocyanide.

## CHE C11: CHEMISTRY ELECTIVE LAB-3

### Physical Chemistry group

- A. Chemical Kinetics**
  - Determining the energy of activation and entropy of activation in KMnO<sub>4</sub>-benzyl alcohol reaction measuring the rate constant at least at three temperatures.
  - Determining the Formation Constant for the [Ce<sup>+4</sup>-H<sub>3</sub>PO<sub>2</sub>] intermediate complex and also the rate constant of its decomposition.
  - Determine the rate constant in bleaching of malachite green in the basic medium.
- B. Spectrophotometry / Colorimetry**
  - Verify Beer's Law for the solution of potassium permanganate (KMnO<sub>4</sub>) and determine the concentration of the given aqueous solution of unknown concentration of this salt.
  - Determine the pH of the solution employing methyl red indicator spectrophotometrically.
  - Determine indicator constant (pK<sub>a</sub>) of methyl red, spectrophotometrically.
  - Determine stability constant of FeSCN<sup>+2</sup> complex ion spectrophotometrically keeping strength constant.
- C.**
  - Determination of Solubility of various salts like NaCl, KCl, KNO<sub>3</sub> and NaNO<sub>3</sub> at different temperature and draw the solubility Curve.
  - Study the variation of viscosity of pure liquid with temperature and determination of temperature coefficient of viscosity of the liquid.
  - Determination of Glass transition temperature of a given salt (e.g., CaCl<sub>2</sub>) conductometrically.
  - Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.

## CHE D11: CHEMISTRY ELECTIVE LAB-3

### Organic group

#### Multi-step Organic synthesis based on Name Reactions

The exercise should illustrate the use of organic reagents and purification of products by chromatographic techniques.

- i. Photochemical reaction :  
(Benzophenone → Benzpinacol → Benzpinacolone)
- ii. Beckman Rearrangement : Benzanilide from benzene  
(Benzene → Benzophenone → Benzophenone oxime → Benzanilide)
- iii. Benzilic acid rearrangement : Benzilic acid from benzoin  
(Benzoin → Benzil → Benzilic acid).
- iv. Synthesis of heterocyclic compounds
  - a. Skraup synthesis: Preparation of quinoline from aniline
  - b. Fisher Indole synthesis: Preparation of 2-phenylindole from phenylhydrazine.
- v. Diazocoupling: Phthalic anhydride → Phthalamide → anthranilic acid → methyl red.
- vi. More Name reaction based organic synthesis based on curricula may be added

## CHE E11: CHEMISTRY ELECTIVE LAB-3

### Pharmaceutical Chemistry group

- i. Identification reactions of ions such as aluminium, ammonium salts, arsenic, calcium and sodium chloride.
- ii. Limit tests of ammonium, fluorides, magnesium, heavy metals and iron
- iii. Assay of Hydrogen Peroxide Solution and Isolation of Bismuth from Pepto-Bismol
- iv. The Isolation of Lactose from Milk
- v. Assay for Galacturonic Acid
- vi. Separation of Fatty Acids and Glycerol and Extraction of Glycerol
- vii. Color Reactions of Proteins - Biuret Reaction, Ninhydrin Reaction, Xanthoproteic, Ehrlich Diazo Reaction
- viii. Enzyme Activity and Intestinal Digestion.
- ix. Preparation of cyclic nucleotide, Isolation of RNA.

#### Books suggested

1. Experiments in Pharmaceutical Chemistry, Second Edition, Charles Dickson, CRC Press
2. Pharmaceutical Chemistry I - laboratory Experiments and Commentary, Attila Almasi et.al, EU Social Fund Project

## EoSE of CHEMISTRY CORE / ELECTIVE LABORATORY COURSE

DURATION: 6 Hrs MAX. MARKS: 100

Practical Exercises	75 Marks (three each of 25 marks)
Practical Record	10 Marks
Viva	15 Marks

**CHE X01: SOLID STATES AND NANOMATERIALS**

**4 Credit (4 hrs/week)**

**UNIT-I**

**Solid State Chemistry**

Introduction to the solid state, defects of solids, classification of imperfections, Electronic defects, atomic defects, Lattice imperfections, thermodynamics of Schottky defect and Frenkel defect. Electrical, optical, magnetic and thermal properties of inorganic materials.

**Solid State Reactions:** general principles, types; sintering; nucleation; Factors influencing the reactivity of solids; co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

**UNIT-II**

**Superconductors**

Superconductors, with special emphasis on the synthesis and structure of high temperature superconductors; solid state LASERS (Ruby, YAG and tunable lasers): Inorganic phosphor materials; synthesis and advantages of optical fibers over conducting fibres, diffusion in solids, catalysis and zone refining of metals.

**UNIT-III**

**Diffraction Methods**

**A. X-ray Diffraction**

Bragg condition, Miller indices, Laue Method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern, Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem; description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

**B. Electron Diffraction**

Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules, low energy electron diffraction and structure of surfaces.

**UNIT-IV**

**Nanomaterials**

Various preparative approaches and techniques; characteristic differences of nanomaterials over bulk materials; dynamic light scattering, atomic force microscopy and characterization of nanomaterials; imaging techniques: electron microscopy (Scanning Electron Microscopy, Transmittance Electron Microscopy). Applications of nanomaterials.

**SUGGESTED BOOKS AND REFERENCES**

4. H.V. Keer, Principles of the Solid State; Wiley Eastern Ltd.: New Delhi, 1993.
5. A.R. West, Solid State Chemistry and its Applications; 2<sup>nd</sup> Edn, John Wiley and Sons, 2014.
6. N. B. Hannay, Treatise on Solid State Chemistry; Plenum, 1976.
7. A. K. Cheetham and P. Day, Eds. Solid State Chemistry Techniques; Clarendon Press, Oxford, 1987.
8. John Wulff, The structure and properties of materials, John Wiley & Sons: Trans edition, 1966.
9. L. V. Azaroff, J. J. Brophy, Electronic processes in materials, Mc Craw Hill, 1967.
10. D. K. Chakrabarty, Solid State Chemistry, New Wiley Eastern, 2009.
11. M.C. Day, J. Selbin, Theoretical Inorganic Chemistry, Reinhold Publishing, New York, 1962.
12. A.W. Adamson and A.P. Gast, Physical Chemistry of Surfaces, Wiley-Interscience; 6<sup>th</sup> Ed 1997
13. G. Timp, Ed. Nanotechnology, Springer-Verlag, N. Y., 1999.
14. B. D. Eshleman, Materials Chemistry, Springer, 2007.

## UNIT-I

**Retrosynthetic Analysis**

An introduction to synthons and synthetic equivalents. Disconnection approach, good disconnections, functional group inter-conversions, importance of the order of events in organic synthesis. One group C-X disconnections. Chemoselectivity. Two group C-X disconnections.

Reversal of polarity (Umpolung), generation of acyl anion equivalent-1,3-dithiane from carbonyl compounds, use of methylthio-methylsulfoxide via cyanide ion and cyanohydrin ethers, nitro compounds and metallated vinyl ethers.

Protecting Groups: Principle of protection of carbonyl, hydroxyl, amino and carboxyl groups.

Enamines: Preparation and synthetic applications

## UNIT –II

**One Group C-C Disconnections**

One group C-C disconnection involving alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes, aliphatic nitro compounds in organic synthesis.

**Two group C-C Disconnections**

Diels-Alder reaction. 1,3-Difunctionalised compounds;  $\alpha,\beta$ -unsaturated carbonyl compounds; control in carbonyl condensation; 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

1,2-Difunctionalised compounds. Radical reactions in synthesis. 1,4-Difunctionalised compounds. Reconnections. 1,6-Difunctionalised compounds.

## UNIT III

**Ring Synthesis**

Introduction to ring synthesis of saturated heterocycles. General strategy and stereoselectivity. 3-Membered rings from cyclisations and insertion reactions. Rearrangements in synthesis. 4-Membered rings from photocycloadditions and use of ketenes.

Five-membered rings from 1,4- and 1,6-dicarbonyl compounds. Pericyclic rearrangements and special methods. 6-Membered rings from carbonyl condensations, Diels-Alder reactions and reduction of aromatic compounds. Synthesis of aromatic Heterocycles.

## UNIT IV

**Asymmetric Synthesis**

Concepts of prochirality, enantioselectivity and diastereoselectivity. Methods for determination of enantiomer purity. Stereogenic skeletal bond forming reactions. synthesis of a racemate and resolution. Asymmetric synthesis, enantiomeric excess. chiral pool, chiral auxiliaries, chiral reagents and chiral catalysts.

**Organic Transformations by C-H functionalization**

Introduction to C-H Activation and C-H functionalization, Transition metal catalyzed C-C bond and C-X bond formation *via* C-H functionalization. Metal free organic transformations *via* C-H functionalization.

**SUGGESTED BOOKS AND REFERENCES**

1. Smith M B., Organic synthesis, McGraw Hill, 2002
2. Warren S. & Wyatt P., Organic synthesis: The disconnection approach 2<sup>nd</sup> edn., John Wiley & Sons, 2008.

3. Warren S, Wyatt P, Workbook for Organic Synthesis: The Disconnection Approach, 2nd edn., John Wiley & Sons, 2009. ISBN: 978-0-470-71227-6
4. Warren S., Designing organic synthesis: The synthon approach, Wiley, 1978 (Reprinted 2002).
5. Jonathan Clayden, Nick Greeves, Stuart Warren and Peter Wothers, Organic Chemistry, Oxford University Press, 2001.
6. Fuhrhop J and Li G, Organic Synthesis – Concepts, Methods and Starting Materials, Wiley-VCH, 2003.
7. Kalsi P S, Organic synthesis through disconnection approach, Scientific International, 2014
8. Carruther W., Modern Methods of Organic Synthesis, Cambridge University Press, 2004.
9. House H.O., Modern Synthetic Reactions: Organic chemistry monograph series, W.A. Benjamin, 1972.
10. Xiao-Feng Wu, Transition Metal-Catalyzed Heterocycle Synthesis via C-H Activation, Wiley, 2015. ISBN: 978-3-527-33888-7.



## CHE B04: ADVANCED BIOINORGANIC CHEMISTRY

4 Credit (4 hrs/week)

### UNIT-I

#### **Metalloenzymes:**

Structure and functions of the following enzymes: carbonicanhydrase, carboxypeptidase, alcoholdehydrogenase, catalase and peroxidase, cytochrome P-450, super oxide dismutase and xanthin oxidase, coenzyme, vitamin B12.

### UNIT-II

#### **Metal Storage and Transport:**

Iron storage and transport for mammalia systems, transferrin, ferritin, Transport of iron in microorganism, siderophores, types of siderophores - The catecholate siderophores (eg: enterobactin) and hydroxamate siderophores (eg: ferrichrome), Mechanism involved in binding of Iron(III) siderophores complexes to receptors and the release of Iron into the Cytoplasm. Other storage & transport systems: ceruloplasmin and serum albumin for copper, metalothioneins and phytochepatins.

### UNIT-III

#### **Metal/Nucleic Acid Interactions**

Metal complexes of polynucleotide, nucleosides and nucleic acids (DNA and RNA), Fundamental interactions with nucleic acids, Fundamental reactions of transition metal complexes with nucleic acids, Applications of different Metal Complexes that bind nucleic acids.

### UNIT-IV

#### **Metal Deficiency and Diseases:**

Iron, zinc and copper deficiency, metal ion toxicity, copper over load and Wilson's disease, iron toxicity, toxicity of arsenic, cadmium, mercury and lead, metal complexes in medicine – chelation therapy – BAL, penicillamine, polyamino carboxylic acids and desferrioxamine – gold compounds and rheumatoid arthritis – platinum complexes as anticancer, drugs – metal complexes in radio diagnosis and magnetic resonance imaging.

#### **SUGGESTED BOOKS AND REFERENCES**

1. S. J Lippard & J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books.
2. S. J. Lippard, Progress in Inorganic Chemistry, Vols. 18 and 38, Wiley-Interscience.
3. I Bertini, H.B. Gray. S.J. Lippard and J. S. Valentine, Bioinorganic Chemistry, University Science Books.
4. G.L. Eichhorn (Ed.), Inorganic Biochemistry Vols I and II Elsevier.

## CHE B05 – MATERIALS AND INDUSTRIAL CHEMISTRY

4 Credit (4 hrs/week)

### UNIT – I

**Industrial Chemistry :** Ferrous and non-ferrous metal industries - quality control methods, general principles applied in studying an industry; manufacture of iron, steel and alloy steels; introduction to metallurgy; metallurgy of iron, aluminium, copper, gold and silver; contaminants; waste management; recycling and pollution control; deformation in metals; modes of failure analysis; an overview of corrosion & its protection; industrial shaping of metals.

### UNIT –II

**Cement :** Classification of cement, manufacture of portland cement, setting and hardening of cement, chemical constitution of portland cement and their characteristics, special cements and their uses, Cement Industries in India.

**Ceramics :** Classification of ceramics, basic raw materials, manufacture and applications, components imparting colours, comparison of pottery porcelain and china ware. Glass-raw materials, manufacture and applications: special glass, optical, borosilicate, flint and coloured glasses.

### UNIT III

#### Chemistry of Selective Materials

Solid electrolytes: AgI,  $\text{RhAg}_4\text{I}_5$ ,  $\beta$ -Alumina – NASICON – Principles and Applications of solid electrolytes.

Ferroelectric, piezoelectric and pyroelectric materials – principle, properties and applications. LED – principle – types – advantages and disadvantages of LED displays

Liquid crystal display LCD – properties – twisted nematic field display – Advantages and disadvantages of LCD – comparison of LCD & LED.

Shape Memory alloys (SMA) – classification – working principles. Non-linear optical materials – second harmonic generators

### UNIT IV

**Chemistry of Inorganic Materials :** Refractories – characterization properties and applications. Microscopic composites; dispersion strengthened and particle – reinforced, fibre- reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties and applications.

### SUGGESTED BOOKS AND REFERENCES

1. Harold H. Trimm, William Hunter III, Harold Henry Trimm, Industrial Chemistry: New Applications. Processes and Systems, Apple Academic Press, Inc., 2011
2. Fontana and Greene, Corrosion Engineering: McGraw Hill Publication, 1986.
3. E. Stocchi, Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK, 1990.
4. R.M. Felder, R W Rousseau, Elementary Principles of Chemical Processes. Wiley, New Delhi.
5. George Austin. Shreve's Chemical Process Industries, McGraw-Hill Book Company, 1985.
6. R.M.E. Diamant, Applied Chemistry for Engineer, Pitman Publishing, 3<sup>rd</sup> Edition, 1972.
7. Alan Heaton, An Introduction to Industrial Chemistry, Springer, 1996.
8. R.N. Shreve, "Chemical process industries", McGraw-Hill, Kugakuisha Ltd., Tokyo, 1984.
9. Riegels Hand Book of Industrial Chemistry. 9th edition. J.A. Kent (Ed), New York, 1992
10. J.A. Kent, Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
11. Mark Anthony Benvenuto, Industrial Chemistry, de Gruyter GmbH, 2013.
12. S.S. Dara, S.S. Umare, A Textbook of Engineering Chemistry, S. Chand & Company Ltd. New Delhi. 2013.
13. Study Material in vocational subject, Industrial Chemistry (UGC Sponsored).



## CHE B06: PHOTOINORGANIC CHEMISTRY

4 Credit (4 hrs/week)

### UNIT-I

#### Basic Concept

Introduction, Photochemical laws and photochemical kinetics. Physical properties of the electronically excited molecules; Photophysical processes in electronically excited molecules

### UNIT-II

#### Photophysical Properties

Photophysical kinetics of Biomolecular processes; kinetics of collisional quenching: Stern-Volmer Equation, Concentration dependence of quenching and excimer formation, charge transfer mechanism and energy transfer mechanism.

### UNIT-III

#### Photochemical Reactions

Photoelectrochemistry of excited state redox reactions. Photosensitization. Types of Photochemical reactions; substitution, decomposition and fragmentation, rearrangement, and redox reactions, photochemistry of metallocenes.

### UNIT-IV

#### Redox Reactions by Excited Metal Complexes

Redox reactions of metal complexes in excited states, excited electron transfer, examples using  $[\text{Ru}(\text{bpy})_3]^{2+}$  complex and  $[\text{Fe}(\text{bpy})_3]^{3+}$  complex. Role of spin-orbit coupling, life-times of excited states in these complexes.

**Metal Complex Sensitizers:** Electron relay, semiconductor supported metal oxide systems, water-photolysis, nitrogen fixation and carbon dioxide reduction.

#### SUGGESTED BOOKS AND REFERENCES:

1. K.K.Rohatagi-Mukherjee, Fundamentals of Photochemistry, Wiley Eastern, 1986
2. A.W. Adamson and P.D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, NY, 1975.
3. G.L.Geoffrey and M.S. Wrighton, Organometallic Photochemistry, Academic Press, 1979.
4. Inorganic Photochemistry, J. Chem. Educ. vol. 60 No. 10, 1983.
5. Coordination Chem. Revs., vol. 39, 121, 1231, 1981; 14, 321, 1975; 97, 313, 1990.
6. V. Balzari and V. Carassiti, Photochemistry of Coordination Compounds, Academic Press, 1970.
7. G.J. Ferraudi, Elements in Inorganic Photochemistry, Wiley, NY, 1988.
8. S.J. Lippard, ed., Progress in Inorganic Chemistry, Vol. 30. Wiley, 2009.

## UNIT - I

**Induced Phenomena:**

Induced reactions, kinetics of Induced reactions and their characteristics. Induction factor and its mechanistic significance. Mechanism of –

- (i) Fe (II) induced oxidation of iodide by Cr (VI).
- (ii) As (III) induced oxidation of Mn (II) by chromate in acid solutions.
- (iii) Kinetics and mechanism of induced reactions in metal complexes (octahedral complexes of cobalt (III) only).

## UNIT II

**Metal-ion Catalysis: Kinetics and Mechanism of following Reactions**

- (i) When reaction rate is independent of one of the reactants in presence of metal ion catalyst.
- (ii) When reaction rate is retarded by one of the products in presence of metal ion catalyst.
- (iii) When metal ion catalysis indicates an intermediate species.
- (iv) Cyclodextrines are acting as catalyst mode of catalysis. Analysis of one full case study of B-cyclodextrine, catalysed reaction, Hydroformylation reaction

## UNIT – III

**Oscillatory Reactions:** Autocatalysis and oscillatory reactions, thermodynamics approach of oscillatory reactions, Kinetics and mechanism of Belousov-Zhabotinski (B-Z) reaction

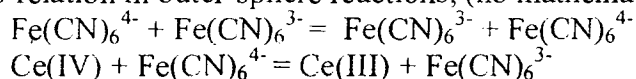
**Substitution Reaction:** Classification of ligand substitution reaction, Kinetics and mechanism of Anation reaction, base catalyzed reaction and acid catalyzed reaction. Kinetics and mechanism of 1:1, 1:2 and 1:3 metal-substrate complexes as intermediates.

## UNIT – IV

**Electron Transfer Reactions in Metal Complexes:**

Inner-sphere and outer-sphere reactions, Mechanism of inner sphere and outer sphere mode of electron transfer reactions. Henry Taube's classical reaction, its kinetics and mechanism, experimental analysis by chromatographic and spectroscopic techniques. Pattern of reaction via adjacent and remote attacks, linkage isomerism.

Marcus -Cross-relation in outer-sphere reactions, (no mathematical derivation) in following reactions-



Bridged outer-sphere electron transfer mechanism.

**SUGGESTED BOOKS AND REFEREN**

1. Henry Taube, S Lippard (Ed.), Progress in Inorganic Chemistry, Vol 30. John Wiley & Sons, NY, 1983.
2. R. Lumry and R.W. Raymond, Electron transfer reaction, Inter-Science Publication, 1997.
3. N. I. Bender, Mechanism of homogeneous Catalysis from protein to protein, Wiley, 1971.
4. A. G. Sykes, Kinetics of Inorganic reactions, Pergamon Press, 1966.
5. S. W. Benson, Jacob Kleinberg, R. Kent Murmana, R. T. M. Fraser, John Bauman, Mechanism of Inorganic Reactions, Academic Press, 1965.
6. H Taube, Electron transfer reactions in solution, Academic Press, London, 1970

UNIT-I

**Electrochemical analysis**

Introduction to electrochemical methods, electrochemical cells, diffusion controlled limiting current, voltage scanning polarography, shape and interpretation of polarographic wave, current –voltage relationship during electrolysis. General Principle and applications of Linear Sweep Voltammetry (LSV), Cyclic Voltammetry (CV), Square Wave Voltammetry (SWV), and Differential pulse Voltammetry (DPV). Stripping voltammetry: Principle, classification and Applications.

UNIT-II

**Electro-catalysis**

Chemical catalysis and Electro-catalysis, cathodic and anodic electro catalysis; electrocatalysis of mixed oxides of titanium doped with rare earth oxides (Ebonex); Electrolysis in simple redox reactions. Electrocatalysis of bimetallic nanostructured materials.

Photoelectrochemistry: introduction, Principle of photoelectrochemistry, types of photoassisted redox reaction, organic photo-electrochemical reactions. Examples of some abnormal electro-organic synthesis.

UNIT-III

**Electro-organic Synthesis**

Types of electro organic reactions, constant current and constant potential electrolysis, cell design, effect of variable, nature of medium, nature of electrode materials, over-voltage, effect of redox couple, application to sewage waste water treatment, electro-chemical incineration of human waste in combined space. Electro-organic synthesis of novel drugs.

UNIT-IV

**Electrochemical Sensors**

Electrochemical Sensors for Nitric Oxide (NO), pesticides, glucose and superoxide species, Electrochemical sensors based on carbon nano tubes and their applications.

**Energy Options:** Hydrogen Economy, Introduction, Hydrogen Production, Hydrogen Transmission, storage and distribution, Hydrogen fueled equipments, local electricity production from hydrogen, Hazards and safety aspects of hydrogen.

**SUGGESTED BOOKS AND REFERENCES**

1. Joseph Wang, Analytical Electrochemistry, Wiley-VCH Publication, 1998.
2. Zhang, Ju and Joseph Wang, Electrochemical Sensors, Biosensors and their Bio-medical Applications, Academic Press, Elsevier, 2008.
3. A. J. Fry and W. E. Britton, Topics in Organic Electrochemistry, Plenum publishing press. New York, 1981.
4. Baizer Organic Electrochemistry, Marcel Dekker Press, 1980.
5. D K Sharma, Electrochemical Incineration of human waste in confined Spaces, Lambert Publication, Germany, 2012.
6. Bockris and Reddy, Modern Electrochemistry, Volume 2A & 2B, Springer.
7. Brett and Brett, Electrochemistry: Principle and Applications. Oxford Press, 2005.

## CHE C06: ADVANCED NANOSCIENCE AND NANOTECHNOLOGY

4 Credit (4 hrs/week)

### UNIT-I

#### **Nanoscience and Nanotechnology**

Basic concepts of Nano science and technology, Quantum wire, Quantum well, Quantum dot, Properties and technological advantages of Nano materials, Material processing by Sol, Gel method, Chemical Vapour deposition and Physical Vapour deposition methods

### UNIT II

#### **Synthesis**

Top-down (Nanolithography, CVD), Bottom-up (Sol-gel processing, chemical synthesis). Wet Deposition techniques, Self-assembly (Supramolecular approach), Characterization TEM, SEM and SPM technique, Fluorescence Microscopy and Imaging.

Use of bacteria, fungi, Actinomycetes for nanoparticle synthesis, Magnetotactic bacteria for natural synthesis of magnetic nanoparticles; Viruses as components for the formation of nanostructured materials; Synthesis process and application, Role of plants in nanoparticle synthesis.

### UNIT III

#### **Nanoscale Carbon**

Introduction –Carbon molecules-nature of the carbon bond-new carbon structures-discovery of C60-structure of C60 and its crystal- From a Graphene Sheet to a Nanotube, Single wall and Multi walled Nanotubes, Zigzag and Armchair Nanotubes, Euler's Theorem in Cylindrical and Defective Nanotubes.

History Molecular and Super molecular Structure-Intrinsic properties of individual carbon nano tubes-Synthesis -Arcing in the present and absent of catalyze-laser method-Chemical Vapour Deposition - ball milling.

### UNIT IV

#### **Applications**

Solar energy conversion and catalysis, Polymers with a special architecture, Liquid crystalline systems, Applications in displays and other devices, Advanced organic materials for data storage, Photonics, Plasmonics, Chemical, electrochemical and biosensors, Nanomedicine, Nanofoods, Nanocosmetics and Nanobiotechnology.

### SUGGESTED BOOKS AND REFERENCES

1. B. Vishwanathan, Nano materials, Narosa Publication, 2009
2. Foster Lynn E, Nanotechnology, Pearson education, 2005.
3. T. Varghese and K M Balakrishna, Nanotechnology, Thomas Atlantic Publication, 2005.
4. J.J. Ramsden, Nanotechnology: An Introduction, Elsevier Publication, 2004.
5. B.K. Parathasarathy, An Introduction to Nanotechnology, Isha publication, 2007.
6. K.K. Chattopadhyay, Introduction to Nanoscience and Nanotechnology, PHI Publication, 2009.
7. Frank Owens, Introduction to Nanotechnology, Wiley, 2007.

## CHE D05: HETEROCYCLIC CHEMISTRY – II

4 Credit (4 hrs/week)

### UNIT – I

**Five-membered Heterocycles with more than two Heteroatoms:** Synthesis and reactions of triazoles, tetrazoles, oxadiazoles, thiadiazoles and diazaphospholes.

**Meso-ionic Heterocycles:** General classification, chemistry of some important meso-ionic heterocycles of type A and B and their applications.

### UNIT –II

**Six-Membered Heterocycles with one Heteroatom:** Synthesis and reactions of pyrylium salts, pyrones, coumarins, chromones and phosphorine (phosphabenzene).

**Six-Membered Heterocycles with two or more Heteroatoms:** Synthesis and reactions of diazines, triazines, tetrazines and azaphosphorine.

### UNIT –III

Oxazines, Benzoxazines; synthesis and reactions.

Thiazines, 1,4-benzothiazines and phenothiazines; synthesis and reactions.

Diazepines, 1,4- or 1,5-benzodiazepines; synthesis and reactions.

Thiazepines, 1,4- or 1,5-benzothiazepines; synthesis and reactions.

### UNIT-IV

#### Large membered heterocycles

Eight-membered : 1-Azocine, Diazocine, synthesis and reactions.

Nine-membered : 1-Azonine, 2-Oxonine, synthesis and reactions.

Ten or large membered rings, synthesis and reactions.

#### SUGGESTED BOOKS AND REFERENCES

1. R.R. Gupta, M. Kumar and V. Gupta, Heterocyclic Chemistry Vol 1-3, Springer Verlag, 1998, 1999 & 2006.
2. T Eicher and S. Hauptmann, The Chemistry of Heterocycles. Wiley-VCH, 2003.
3. J.A. Joule, K. Mills and G.F Smith, Heterocyclic Chemistry, Chapman and Hall, 1995.
4. T.L. Gilchrist, Heterocyclic Chemistry, Longman Scientific & Technical, 1992.
5. G.R. Newkome and W. W. Paudler, Contemporary Heterocyclic Chemistry. Wiley Inter Science, 1982.
6. A.R. Katritzky & C W Rees (eds), Comprehensive Heterocyclic Chemistry, Pergamon Press, 1934.

## UNIT-I

**Biosynthesis of natural products**

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods.

Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway: Biosynthesis of terpenes – mono, sesqui, di, tri ( $\beta$ -amyrin) and carotenoids, steroids – cholesterol.

## UNIT-II

**Synthesis of Some Natural Products**

Approaches to prostaglandin synthesis; Woodward synthesis of PGF<sub>2a</sub>, Corey's synthesis of prostaglandins E and F. Synthesis Tetrahydroisoquinoline alkaloids. Synthesis of Taxol. Asymmetric Synthesis of  $\alpha$ -Amino Acid.

## UNIT-III

**Design and synthesis of analogues of natural products**


Introduction, diverted total synthesis (DTS), function-oriented synthesis (FOS), biology-oriented synthesis (BIOS), complexity to diversity (CtD), hybrid molecules, and biosynthesis inspired synthesis. The latter includes mutasynthesis, the synthesis of natural products encoded by silent genes, and propionate scanning

## UNIT-IV

**Chemistry of Natural Products:** such as carbohydrates, proteins and peptides, fatty acids, nucleic acids and Lipids.

**SUGGESTED BOOKS AND REFERENCES**

1. J. Mann, Secondary Metabolism, 2nd Edition Oxford University Press, 1987.
2. J. Mann, Chemical aspects of Biosynthesis, Oxford University Press, 1995.
3. I. L. Finar, Organic Chemistry: Vol. 1 & 2. ELBS, Longman, 1996.
4. R. O. C. Norman and J. M. Coxon, Principles of organic synthesis, Chapman and Hall, 1993.
5. Fieser and Fieser, Steroids, Literary Licensing, LLC, 1959.
6. P. Yates, W.A. Benjamin, Structure Determination. Inc., New York, 1967.
7. P. Manitto, Biosynthesis of Natural Products. John Wiley & sons, 1981.
8. K. C. Nicolaou & E. J. Sorensen, Classics in Total Synthesis. Wiley-VCH, 1996.
9. Jonathan Clayden, Nick Greeves, Stuart Warren and Peter Wothers, Organic Chemistry, Oxford University Press, 2000.
10. P. S. Kalsi, Chemistry of Natural Products. Kalyani Publishers/Lyall Bk Depot, 2001.
11. Monroe E. Wall, M. C. Wani, C. E. Cook, Keith H. Palmer, A. T. McPhail, G. A. Sim, Plant Antitumor Agents. I. The Isolation and Structure of Camptothecin, a Novel Alkaloidal Leukemia and Tumor Inhibitor from Camptotheca acuminata. J. Am Chem. Soc. 88. 3888-3890, 1966
12. M. C. Wani and M. E. Wall. Plant antitumor agents. The structure of two new alkaloids from Camptotheca acuminata. J. Org. Chem. 34. 1363, 1969

  
 Dy. Registrar  
 (Academic)  
 University of Rajasthan  
 JAIPUR

13. R. Misra, R. C. Pandey, Sukh Dev, The chemistry of the oleo resin from *hardwickia pinnata*: a series of new diterpenoids, *Tetrahedron Letters*, 3751, 1964; (ii) R. Carrington, G. Shaw, D.V. Wilson, Use of 5-phospho- $\beta$ -D-ribosyl azide in a new direct synthesis of nucleotides, *Tetrahedron Letters*, 2861, 1968.
14. *J.C.S. Perkin Transactions II*, 288-292, 1973; (ii) *J. Am. Chem. Soc.* Vol.77.432-437, 1955.
15. Martin E. Maier, Design and synthesis of analogues of natural products, *Org. Biomol. Chem.*, 13, 5302, 2015.
16. Robert M. Williams, Natural Products Synthesis: Enabling Tools To Penetrate Nature's Secrets of Biogenesis and Biomechanism, *J. Org. Chem.*, 76, 4221-4259, 2011.
17. Mirna Leonor Sua' rez-Quiroz *et al.*, Isolation of green coffee chlorogenic acids using activated carbon, *Journal of Food Composition and Analysis* 33, 55-58, 2014.

## UNIT-I

**Antineoplastic agents** : Introduction to cancer chemotherapy, Classification of antineoplastic agents, role of alkylating agents and antimetabolites in treatment of cancer. Carcinolytic antibiotics and mitotic inhibitors. Synthesis of Cyclophosphamide, Melphalan, Fluorouracil. Recent development in cancer chemotherapy.

**Local Antiinfective drugs** : Introduction. Synthesis and general mode of action of Furazolidone, Ciprofloxacin, Dapsone, Isoniazid, Fluconazole. Antimalarials: Synthesis and general mode of action of Chloroquin.

## UNIT-II

**Cardiovascular Drugs** : Introduction, Classification and general mode of action, Cardiovascular disease, drug inhibitors of peripheral sympathetic function. Synthesis of Sorbitrate, Diltiazem, Verapamil, Methyldopa, Atinlol.

**Diuretics** : Introduction, Classification and general mode of action, Synthesis of Acetazolamide, Chlorothiazide, Frusemide, Spironolactone, Triamterene.

**Hypoglycaemic Agents** : Introduction, General mode of action, Insulin and insulin preparations, Oral hypoglycemic agents: Classification, Synthesis of Tolbutamide.

## UNIT-III

**Psychoactive drugs** : Introduction, Neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, antianxiety drugs.

**Anticonvulsant Drugs** : Introduction, Classification and general mode of action, synthesis of Phenytoin sodium, Troxidone, Ethosuximide, Primidone.

**Antiviral Drugs** : Introduction, Classification and general mode of action, synthesis of Amantadine Hydrochloride, Idoxuridine. Methisazone.

## UNIT-IV

**Antibiotics** : Antibiotics inhibiting protein synthesis,  $\beta$ -lactam rings. Synthesis of Penicillin-G, Ampicillin, Amoxycillin. Chloramphenicol, Cephalosporin, Tetracyclin and Streptomycin.

**Antihistamines** : Introduction, Classification and general mode of action, Synthesis of Pheniramine, Promethazine, Ranitidine, Sodium Cromoglycate.

**Analgesics and Antipyretics** : Classification, Nonnarcotic analgesic. Synthesis of Mefenamic acid, Diclofenac.

## SUGGESTED BOOKS AND REFERENCES

1. J. Stringer, Basic Concepts in Pharmacology (3<sup>rd</sup>edn.), McGraw-Hill Professional, 2005.
2. B. Katzung. Basic and clinical pharmacology (11<sup>th</sup>edn.), McGraw-Hill medical, 2009.
3. A. Burger, M.E. Wolff, Medicinal Chemistry and Drug Discovery, Vol-1, John Wiley, 1994.
4. Goodman & Gilman. Pharmacological basis of Therapeutics, McGraw-Hill, 2005.
5. S.S. Pandeya & J.R Dimmock, Introduction to drug design, New Age International, 2000.
6. A. Kar, Medicinal Chemistry, New Age International, 2007.
7. H. Singh & V. K. Kapoor, Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan New Delhi, 2001.
8. D. Ledwith. Strategies for organic drug Synthesis and Design, John Wiley, 1998.
9. A. Gringauz. Introduction to Medicinal Chemistry: How drugs act and Why? John Wiley and Sons, 1997.
10. Graham and Patrick, Introduction to medicinal Chemistry (3<sup>rd</sup>edn.), OUP, 2005.



**Unit I**

**Dosage Form Design**

Need for dosage form, General considerations for dosage form design, Definition and types of pharmaceuticals ingredients and excipients, Flavouring, sweetening and colouring pharmaceuticals, Preservatives -sterilization and preservation, preservative selection, general consideration, and mode of action

**Unit II**

**Solid Modified –Release Drug Delivery System**

Rationale for extended release pharmaceuticals, Drug candidates for extended-release products, Extended-release technology for oral dosage forms, Delayed- release oral dosage forms.

**Transdermal drug delivery systems**

Transdermal drug delivery systems- introduction, factors affecting percutaneous absorption, percutaneous absorption enhancers, Advantages and disadvantages of TDDSs

**Unit III**

**Novel Dosage Forms**

Novel drug delivery systems- introduction and composition, Iontophoresis (IP) and phonophoresis, Mucoadhesive system, Medicated gums, Intravaginal drug delivery system, Intrauterine progesterone drug delivery system , Bioadhesive vaginal gel, Dinoprostone Vaginal Insert, Estring Long-acting parenteral systems, Liposomes as drug delivery vehicles

**Unit IV**

**Products of Biotechnology**

Introduction, Techniques for the production of biotechnologic products, Products of biotechnology such as Anticoagulant Drug: Lepirudin (Refludan) Antisense Drugs: Fomivirsen Sodium (Vitravene), Erythropoietins. Epoetin Alfa. Growth Factor: Becaplermin, Human Growth Hormone, Systemic Growth Hormone, Interferons and Interleukins

**BOOKS AND REFERENCES**

1. Organic Medicinal and Pharmaceutical Chemistry, John M. Beale, Jr., John H. Block, Wolters Kluwer
2. Ansel's Pharmaceutical Dosage Forms and Drug Delivery Systems, Loyd V Allen, Wolters Kluwer
3. Drug delivery : principles and applications , Binghe Wang, Teruna Siahaan, Richard soltero, John Wiley & Sons.

## CHE E04: ADVANCED PHARMACEUTICAL CHEMISTRY

4 Credit (4 hrs/week)

### UNIT-I

#### **Biotechnological Applications of Enzymes**

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from crown starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

### UNIT II

#### **Prodrugs Approaches to Drug Delivery**

Introduction, Basic concepts: definition and applications, Prodrug design considerations, Prodrugs of various functional groups- Ester prodrugs of compounds containing -COOH or -OH, Prodrugs of compounds containing amides, imides, and other acidic NH (Mannich bases and N-a-Acyloxyalkyl derivatives, Prodrugs of amines, Prodrugs for compounds containing carbonyl groups

### UNIT III

#### **Radiopharmaceutical:**

Introduction, Background information, Therapeutic use of radiopharmaceuticals, Representative radiopharmaceutical drugs and primary uses, Mode of actions of some important radiopharmaceuticals such as Technetium-99 m, Strontium-89 Chloride, Yttrium-90 and Thallous-201 Chloride.

### UNIT IV

#### **Non radioactive Pharmaceuticals in Nuclear Medicine**

Introduction, Mode of action and use of Acetazolamide, Cimetidine, Dipyridamole Adenosine, Furosemide and Vitamin B12, Practice of nuclear pharmacy, Procurement and storage.

### SUGGESTED BOOKS AND REFERENCES

1. Bioorganic Chemistry: A chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer Verlag.
2. Understanding Enzymes, Trevor Palmer, Prentice Hall.
3. Enzyme Chemistry: Impact and Applications, Ed. Collin J Suckling, Chemistry
4. Drug Delivery: Principles and Applications, BingheWanget.al., Wiley Interscience
5. Pharmaceutical Dosage Forms and Drug Delivery Systems, Loyd V. Allen junior et al., Wolters Kluwel

## CHE B12: CHEMISTRY ELECTIVE LAB-4

### Inorganic Chemistry

Practical Laboratory: 9 hours per week (6 Credit)

Examination: Duration: 6 Hours; Max. Marks: 100

#### A. Quantitative analysis:

- i) Separation and determination of two metal ions involving Volumetric and Gravimetric methods:
  - b. Copper – Nickel
  - c. Copper – Zinc
  - d. Iron– Nickel
- ii) Estimation of sulphate as barium sulphate gravimetrically.
- iii) Estimate Ni in a given sample complexometrically using murexide as an indicator.
- iv) Analysis of the given sample of iron ore & determination of Silica – Gravimetrically, Iron Volumetrically to find out their percentages in the given sample.
- v) Analysis of German silver for copper and nickel.
- vi) Estimation of copper (iodometrically) and zinc (complexometrically by EDTA) in Brass.
- vii) Estimation of Iron in Portland cement.

#### B. Preparation of the following inorganic compounds and their spectroscopic studies.

- i. *Cis-* and *trans-* $K[Cr(C_2O_4)_2(H_2O)_2].2H_2O$
- ii.  $Mn(acac)_3$
- iii.  $R_2Sn(acac)_2$
- iv.  $VO(acac)_2$
- v.  $Na[Cr(NH_3)_2(SCN)_4]$
- vi.  $[Ni(NH_3)_6]Cl_2$

## CHE C12: CHEMISTRY ELECTIVE LAB-4

### Physical Chemistry

Practical Laboratory: 9 hours per week (6 Credit)

Examination: Duration: 6 Hours; Max. Marks: 100

#### A. Electrochemistry

- i. Identification and Estimation of metal ions such as  $Cu^{+2}$ ,  $Cd^{+2}$ ,  $Ni^{+2}$  Voltammetrically.
- ii. To plot a cyclic voltammogram of a reversible system and calculate the number of electron in the redox process.
- iii. To plot a voltammogram of a organic compound (such as nitroaniline, picric acid, m-dinitrobenzene) and verification of Randel Sevcik equation (current vs scan rate and current vs concentration)
- iv. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
- v. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.

#### B. Chemical Kinetics

- i. Determine the order with respect to Ag (I) in the oxidation of Mn (II) by  $S_2O_8^{2-}$  and the rate constant for the unanalyzed reaction.
- ii. Investigate the autocatalysed reaction between  $KMnO_4$  and Oxalic Acid.
- iii. Kinetics of enzyme catalyzed reactions.
- iv. Flowing clock reaction (Ref: Experiments in physical Chemistry by Snowmaker).
- v. Oscillatory reaction

**CHE D12: CHEMISTRY ELECTIVE LAB-4**  
**Organic Chemistry**

**Practical Laboratory: 9 hours per week (6 Credit)**

**Examination: Duration: 6 Hours; Max. Marks: 100**

**Qualitative analysis:** Separation of three component organic mixture and identification of its components, Preparation of their derivatives and verification with the help of IR and NMR spectral data provided.

**CHE E12: CHEMISTRY ELECTIVE LAB-4**  
**Pharmaceutical Chemistry**

**Practical Laboratory: 9 hours per week (6 Credit)**

**Examination: Duration: 6 Hours; Max. Marks: 100**

- i. Identification reactions of functional groups such as Alkaloids, Barbiturates ( non nitrogen substituted, Lactates, Tartrates,
- ii. Pharmacopoeal qualifications of active pharmaceutical ingredients such as chloral hydrate, hexobarbital, caffeine, acetyl salicylic acid, atropine sulphate and quinine hydrochloride
- iii. Preparations of Benzocaine and Acetaminophen
- iv. Assay of Sulfadiazine Tablets and Assay of Amitriptyline HCl
- v. Thiamine Assay of Vitamin B Complex Tablets
- vi. Determination of Vitamin C content of Commercial Tablets
- vii. Study of some colour reactions of Antibiotics

**Books**

- i. Experiments in Pharmaceutical Chemistry, Second Edition Charles Dickson, CRC Press
- ii. Pharmaceutical chemistry I- laboratory Experiments and Commentary, Attila Almasi et.al, EU Social Fund Project

**CHE A13: CHEMISTRY ELECTIVE LAB - 5**

**Practical Laboratory: 9 hours per week (6 Credit)**

**Examination: Duration: 6 Hours; Max. Marks: 100**

**A. Preparation and evaluation of -**

- i. Emulsion, simple syrup
- ii. Aqueous iodine solution, strong iodine solution
- iii. Calamine lotion, boroglycerine
- iv. Peppermint water, rose water, camphor water.
- v. Formulation of magnesium hydroxide mixture (milk of magnesium)

**B. Chemical Analysis and Nanomaterials**

- i. Estimation of Iron in lime stone samples (Marbles).
- ii. Synthesis of ZnO and TiO<sub>2</sub> nanoparticles and their characterization.
- iii. Synthesis of copper conductive paint / ink.
- iv. Synthesis of graphene, graphene oxide (GO) and reduced graphene oxide (rGO)
- v. Study of capping agent of hydrophilic and hydrophobic metal nanoparticles by FTIR.
- vi. Synthesis of different size metal nanoparticles and characterized by UV measurement.

## CIIE A21: PROJECT WORK

**Project Work: 12 Credits (180 hrs)**

**EoSE: Max. Marks: 100**

Project report will be submitted at the end of Project work duly signed by the project guide. The EoSE assessment of the Project Work shall be as per University guidelines.

---

---