Centre for Basic Sciences (CBS) COURSE STRUCTURE SCHEME OF EXAMINATION & SYLLABUS of Five Year

Syllabus of M. Sc. Integrated (Chemistry Stream) UNDER FACULTY OF SCIENCE

Approved by Board of Studies in Chemistry Effective from July 2022 onwards



Center for Basic Sciences Pt Ravishankar Shukla University, Raipur (CG) 492010 Ph. – 077-2262216



# <u>Center for Basic Sciences</u> Pt. Ravishankar Shukla University, Raipur

### **Course structure for the M. Sc. (Integrated) Chemistry stream** Effective from July, 2022

(Abbreviation: B: Biology, C: Chemistry, M: Mathematics, P: Physics, G: General, H: Humanities, BL: Biology Laboratory, CL: Chemistry Laboratory, PL: Physics Laboratory, GL: General Laboratory, PE: Physics Elective, PPr: Physics **Pr**oject)

Subject	Subject	Contact Hours /	Credits		
Code		Week			
		Theory +Tutorials			
B101	Biology – I	[2+1]	3		
C101	Chemistry – I	[2+1]	3		
M101/MB101	Mathematics – I	[2+1]	3		
P101	Physics – I	[2+1]	3		
G101	Computer Basics	[2+1]	3		
H101	Communication Skills	[2]	2		
	Contact Hours /Week Laboratory				
PL101	Physics Laboratory – I	[4]	2		
CL101	Chemistry Laboratory – I	[4]	2		
BL101	Biology Laboratory – I	[4]	2		
GL101	Computer Laboratory	[4]	2		
		(25 of 240 credits)	Total: 25		
Additional Papers					
ES101	Environmental Studies	[2]	2		

### <u>FIRST YEAR</u> SEMESTER –I

#### (25 of 240 credits)

### C 101: Chemistry-I UNIT-I

(30 + 15 = 45 hrs.)

(4 + 2 = 6 hrs.)

### Structure and Properties of atoms: Revisited

(i) Atomic spectra, Bohr's theory of atomic structure, Sommerfield's theory for complex electron spin and magnetic quantum number, Pauli exclusion principle, Hund's rule, electron configuration of elements, Sequence of energy levels and Periodic Table.

(ii) Size of atoms and ions, ionization energy, electron affinity, electronegativity – values by Pauling, Mulliken and Allred-Rochow, Metallic character, variable valency and oxidation states, horizontal, vertical and diagonal relationships in the periodic table.



(iii) Atomic Nucleus: Fundamental particles, classification of nuclides, nuclear stability, the neutron to proton ratio N/Z, nuclear potential, binding energy, exchange force. Radioactivity and radioactive elements, radioactive decay and decay kinetics.

# **UNIT-II**

# **Types of Chemical Bonds**

(i) The covalent bond - the Lewis theory, Octet rule and its limitations, Shapes of the molecules -Sidgwick - powel theory, Valence shell electron pair repulsion (VSEPR) theory, effect of lone pair and electronegativity, isoelectronic principle, examples to apply VSEPR theory, Valence bond theory, Hybridization. Bond length, bond angle & dihedral angle, d-orbital participation in molecular bonding, sigma and pi bonding. Molecular orbital method - Linear combination of atomic orbitals (LCAO), MO treatment for di- and tri-atomic molecules and involving delocalized pi-bonding, Conjugation & aromaticity

# **UNIT-III**

(ii) Metallic bond: theories of metallic bonds, Co-ordinate bond

(iii) Physical properties and molecular structures – polarizability and dipole moments, melting point, solubility and acid-base properties, Intermolecular forces (dipole-dipole interaction) Hydrogen bonding and vander Waals's forces.

### **UNIT-IV**

### **Reactivity & Mechanism:**

(i) Inductive and field effects and bond dissociation energy.  $p\pi$ -d $\pi$  bonding. Delocalization – cross conjugation, resonance. Aromaticity and Huckel's rule – systems of 4n and 4n+2 electrons, Resonance and Hyperconjugation.

(ii) Reaction mechanism: Types of mechanisms, Arrhenius theory, collision theory, types of reactions, redox reactions, displacement and addition reactions, thermodynamic and kinetic requirements.

# **UNIT-V**

(iii)General concepts: Oxidation number and oxidation states, Oxidation – reduction reactions and the use of reduction potential, Bronsted acids and bases, gas phase vs. solution acidity, solvent levelling effects, hardness and softness, surface acidity.

### Suggested texts and References:

(1) J.D. Lee, Concise Inorganic Chemistry, 4th Edition, ELBS, 1991.

(2) P.W. Atkins, Physical Chemistry, Oxford University Press, 7th Edition, 2006.

(3) G.M. Barrow, Physical Chemistry, 5th Edition, Tata McGraw-Hill, New Delhi, 1992.

(4)R. T. Morrison and R. N. Boyd, Organic Chemistry, Prentice Hall of India.

(5)G.W. Castellan, Physical Chemistry, 3rd Ed. Addison - Wesley/Narosa Publishing House, 1993.



#### (12 + 6 = 18 hrs)

### (14+7=18 hrs.)

### CL 101: Chemistry Laboratory

- 1. To calibrate given glasswares (i) 100 ml beaker & (ii) 50 ml volumetric flask.
- 2. To calibrate given glasswares (i) Burette, (ii) Pipette & (iii) Measuring cylinder.
- 3. To calibrate given glasswares (i) Micropipette.
- 4. To determine the strength of unknown solution of NaOH with N/10 oxalic acid by volumetric.
- 5. To determine the strength of unknown solution of NaOH with N/10 hydrochloric acid by volumetric.
- 6. To determine the strength of unknown solution of NaOH with potassium hydrogen phthalate by volumetric.
- 7. To determine hardness of given water sample complexometrically using EDTA & EBT.
- 8. To determine the strength of unknown solution of magnesium salt solution using standard magnesium solution and EDTA complexometrically.
- 9. To identify functional group:
  - (i) Glucose
  - (ii) Starch
  - (iii) Carboxalic acid
  - (iv) Oxalic acid
  - (v) Benzoic acid
  - (vi) Phthalic acid
  - (vii) Acetone
  - (viii) Acetophenone
  - (ix) Methanol
  - (x) Ethanol
  - (xi)  $\beta$  napthol
  - (xii)  $\alpha$  napthol
  - (xiii) Ethyl acetate
  - (xiv) Benzamide
  - (xv) Urea
  - (xvi) Thiourea
- 10. To separate Ni (II) & Co (II) by paper chromatography.

### Suggested text and references:

- (1) Vogel's Textbook of Quantitative Chemical Analysis (5th Edition; Longmann)
- (2) Vogel's Qualitative Inorganic Analysis (7th Edition)
- (3) ACS Journal of Chemical Education









Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
B201	Biology – II	[2+1]	3
C201	Chemistry – II	[2+1]	3
M200/201	Mathematics – II	[2+1]	3
P201	Physics – II	[2+1]	3
G201	Electronics and Instrumentation	[2+1]	3
		Contact Hours / Week Laboratory	
PL201	Physics Laboratory – II	[4]	2
CL201	Chemistry Laboratory – II	[4]	2
BL201	Physics Laboratory – II	[4]	2
GL201	Electronics Laboratory	[4]	2
H201	Communication Skills Lab	[4]	2
	(50 of 240 credits)	Total	25
Additional Paper			
ES201	Environmental Studies	[2]	2

# **SEMESTER –II**

### C 201: Chemistry II UNIT-I

(50 of 240 credits) (30 + 15 = 45 hrs.)

(1) Thermochemistry: Enthalpy, heat of fusion and heat of vapourisation, enthalpy of a chemical reaction (heat of combustion, heat of solution, heat of neutralization), enthalpy of formation, standard reaction enthalpy, Hess's law, Kirchhoff's law, bond energy, dissociation energy. Entropy formulation of Second law, entropy change in a phase transition, Trouton's Rule, calculation of absolute (Third law) entropy, entropy change in a chemical reaction.

### UNIT-II

(2) Free energy functions, criteria for spontaneity and equilibrium of closed systems, variation of Gibbs free energy with pressure and temperature, Gibbs Helmholtz equation, the concept of chemical potential, partial molar quantity, Gibbs Duhem relation.

# UNIT-III

(3) Phase equilibrium in simple systems: Solid – liquid, liquid – vapour, vapour – solid, phase diagrams – water, carbon dioxide, sulphur, phase equilibrium condition, Gibbs phase rule, Clapeyron equations, Clausius – Clapeyron equation.

### UNIT-IV

(4) Ideal Solutions, chemical potential of a solute in a binary ideal solution, Raoult's Law, entropy and Gibbs energy of mixing, Colligative properties – freezing point depression, boiling point elevation, osmotic pressure, van't Hoff equation.



### UNIT-V

(5) Chemical equilibrium: Gibbs energy change of a reaction, standard reaction Gibbs energy, the condition for chemical equilibrium, equilibrium constant, reactions involving gases and pure substances, the Principle of Le Chatelier and applications.

(6) Chemical potential of a charged species, electrochemical cell (galvanic and electrolytic), examples of electrochemical cells, half cell potential (electrode potential), Nernst equation.

### Suggested texts and References:

(1) P.W. Atkins, Physical Chemistry, Oxford University Press, 7th Edition, 2006.

- (2) G.W. Castellan, Physical Chemistry, 3rd Ed.Wesley/Narosa Publishing House, 1993.
- (3) G.N. Lewis and Randall, Thermodynamics, (Revised by K.S.Pitzer and
- L.Brewer), International Students Edition, McGraw Hill, 1961.
- (4) K. Denbigh, The principles of Chemical Equilibrium.
- (5) B. G. Kyle , Chemical & Process Thermodynamics.

### CL 201: Chemistry Laboratory

- 1. To determine endpoint of neutralization by the conductometric titration using strong acid & strong base.
- 2. To determine end point of neutralization by the conductometric titration using weak acid & weak base.
- 3. To determine  $pK_a$  of monobasic acid using pH meter.
- 4. To identify two acidic-, basic- and interfering radicals in given inorganic mixture (various combinations).
- 5. To determine molar volume of isopropyl alcohol & its partial molar volume.
- 6. To determine molar volume of ethanol & its partial molar volume.
- 7. To study the variation of viscosity with ethanol & water.
- 8. To study the variation of viscosity with methanol & water.
- 9. To determine % composition of mixture of ethanol & water by surface tension method.
- 10. To determine % composition of mixture of methanol & water by surface tension method.
- 11. Short project of 2 weeks based on the experiments available in Journal of Chemical Education.

### Suggested text and references:

- (1) Vogel's Textbook of Quantitative Chemical Analysis (5<sup>th</sup> Edition; Longmann)
- (2) Vogel's Qualitative Inorganic Analysis (7<sup>th</sup> Edition)
- (3) ACS Journal of Chemical Education



Contact Hours / Week Theory+Tutorials	Credits
Chemistry [3 + 1]	4
[3+1]	4
[3+1]	4
[3+1]	4
[2+0]	2
Science [2+0]	2
Contact Hours / Week Laboratory	
[6]	3
ratory [4]	2
ts) Total	25

### SECOND YEAR SEMESTER –III

(75 of 240 credits)

# CB 303: Organic Chemistry –I

### (45 + 15 = 60 hrs.)

### UNIT-I

### A. Basic concepts - Recapitulation

Hybridisation, formal charge, inductive and resonance effects and their effect on reactivity and acidity and basicity of organic compounds; polar & non polar covalent bonds; homolytic and heterolytic fission, types of reagents- electrophiles and nucleophiles; curly arrow notation; classification of organic reactions.

### UNIT-II

### **B.** Chemistry of Aliphatic compounds

**IUPAC nomenclature** of aliphatic and substituted aliphatic compounds and alicyclic compounds **Preparation, structure, properties and reactions of the following classes of compounds.** 

i) Hydrocarbons: a) alkanes, Methods of formation Kolbe reaction, Wurtz reaction, Corey House reaction, decarboxylation of carboxylic acids; Mechanism of halogenation of alkanes, orientation, selectivity & reactivity, product ratio. Alkylarenes, preparation via Friedel Crafts reaction. Reactions- oxidation, nuclear and side chain halogenation. b) Cycloalkanes : Methods of formation and reactivity; Baeyer's strain theory and its limitation; theory of strainless rings c) Alkenes: Elimination reactions; Saytzeff & Hoffman elimination; Reactions – halogenation reactions- free radical and polar mechanisms. Markownikoff's rule, the peroxide effect, allylic halogenations using NBS; Ozonides/Ozonolysis. epoxidation; hydroboration-oxidation;



oxymercuration-demercuration; Oxidation using KMnO<sub>4</sub> & OsO<sub>4</sub>.; polymerization. d) **Dienes:** Structure of butadiene and allene ; 1,2 vs 1,4 addition ; Diels Alder reaction.

### UNIT-III

**e)** Alkynes: Methods of formation; acidity of alkynes; electrophilic addition to alkynes; hydroboration oxidation ; metal ammonia reductions; hydrogenation using Lindlar's catalyst.

**ii)** Alkyl halides Preparation, properties and synthetic applications of alkyl halides; SN1 & SN2 reactions (mechanism), E1 and E2 reactions (mechanism); Grignard reagent and its applications. Haloarenes: Preparation, aromatic nucleophilic substitution, elimination-addition and addition-elimination mechanisms, hydrolysis and amination of nitrohaloarenes.

Aromatic electrophilic substitution: General mechanism. Effect of substituents on rate and orientation to aromatic electrophilic substitution in substituted benzenes, ortho-para ratio.

**iii**) **Alcohols:** Methods of formation; acidity; H-Bonding; reactions of mono; di & trihydric alcohols; Diols as protecting groups.

**iv**) **Phenols:** Preparation from sulfonic acids, haloarenes, alkylbenzenes, Acidity, O-alkylation, O-acylation, Fries rearrangement, Claisen rearrangement, Reimer- Tiemann reaction, Hauben Hoesch reaction, Lederer Manasse reaction.

### UNIT-IV

v) Ethers and epoxides: Formation & reactions of ethers and epoxides ; ring opening reactions of epoxides under acidic and basic consitions; reaction epoxides with Grignard & organolithium reagents

vi) Aldehdyes & ketones: Methods of formation of aldehdyes and ketones; Nucleophilic addition reactions with cyanide, ammonia and derivatives of ammonia; acetal formation; oxidation reduction reactions. Meerwin-Pondroff-Verley reduction, Clemmensen reduction, Wolf-Kishner reduction, Aldol condensation reaction, Cannizzaro reaction, Tischenko reaction, haloform reaction, Baeyer-Villiger oxidation, Wittig reaction; Mannich reaction

Aromatic aldehydes and ketones: Preparation via Gattermann, Gattermann-Koch, Vilsmeyer-Haack, Rosenmund and Friedel Crafts acylation reactions, Reactions: Claisen-Schmidt, Knovenagel, Perkin, Benzoin condensation and Cannizaro reactions,

### UNIT-V

vii) Carboxylic acids: Methods of formation of mono and di carboxylic acids; acidity and factors affecting acidity; reactions of carboxylic acids viii) Carboxylic acid derivatives: Methods of formation of acid chlorides, amides, anhydrides and esters and their interconversions; relative stabilities of acid derivatives; Rosenmund reaction; Hoffmann rearrangement; saponification.

Aromatic carboxylic acids: Preparation, acidity, preparation and interconversion of acid derivatives.

**ix**) **Nitrogen and sulphur compounds.** a) Nitro alkanes: methods of formation and reactions of aliphatic and aromatic nitro compounds b) Amines: methods of formation; basicity and factors affecting basicity ; reactions of aliphatic amines. Aromatic nitrogen compounds: Nitro andnitroso compounds - preparation and reduction, Amino compounds – preparation, basicity, Aromatic electrophilic substitution, N-alkylation, N-acylation, Diazotisation, Synthetic uses of diazonium salts, azo coupling c) Sulfonic acids : Methods of formation & reactions of aliphatic sulfonic acids. Aromatic sulfonic acids: Preparation, acidity, preparation and interconversion of sulfonic acid derivatives.

Dr. Sumon Chandworly Mender (Industry Side)

Prof. Goutam Kunnas Patra External member (Acodemics)



### x) Applications of phosphorous and boron in organic synthesis :

Wittig reaction (with mechanism); hydroboration-oxidation (with mechanism); reduction using 9-BBN.

#### Suggested texts and References:

(1) I. L. Finar, Organic Chemistry, Vol. 1 & 2, ELBS.

- (2) R. T. Morrison and R. N. Boyd, Organic Chemistry, Prentice Hall of India.
- (3) J. McMurry, Organic Chemistry, Asian Books Pvt. Ptd.
- (4) L. G. Wade, Organic Chemistry, Pearson Education
- (5) G. Solomons and C. Fryhle, Organic Chemistry, John Wiley & Sons (Asia) Pte Ltd.
- (6) J. March, Advanced Organic Chemistry, 3rd Edn. McGraw Hill, 1991.
- (7) S.H.Pine, Organic Chemistry, 5th Edn., McGraw Hill, 1987.

### C 301: Inorganic Chemistry I

#### UNIT-I

(45 + 15 = 60 hrs.)

(i) Hydrogen: Preparation of hydrogen, Isotopes, ortho and para hydrogen, hydrides.

(ii) **Rare gases:** Occurrence and recovery of the elements, physical and chemical properties, Clathrate compounds, chemistry of Xenon and xenon fluoride complexes.

### UNIT-II

(iii) Chemistry of s-block elements: a) alkali and alkaline earth metals: Extraction, general physical properties, flame colours and spectra, Reaction with water, air and nitrogen, oxides, hydroxides, peroxides and superoxides, sulphides, oxysalts, halides and hydrides, oraganic and organometallic compounds. b) Group IIB elements: Zn, Cd, Hg.

### UNIT-III

(iv) Chemistry of p-block elements: a) Group IIIA elements: Boron, aluminium, gallium indium and thalium – physical properties, oxidation states and type of bonds, Reactions with other elements, compounds of boron with oxygen and hydrogen. b)Group IVA elements: carbon, silicon, germanium, tin and lead – physical properties, allotropesof carbon, graphite compounds, carbaides, carbonates, carbon cycle, silicates, organosilicons, hydrides, halides and cyanides, cluster compounds.

### UNIT-IV

c) Group VA elements: Nitrogen, phosphorous, Arsenic, antimony and bismuth – general properties, hydrides, azides, oxides and oxyacids, sulphides and organometallics, fertilizers.
d) Group VIA elements: oxygen, sulphur, selenium, tellurium and polonium – general properties, structure and allotropy of the elements, chemistry of ozone, oxides, oxyacids, oxohalides, hydrides and halides, organo derivatives.

### UNIT-V

e) Group VIIA elements: Fluorine, chlorine, bromine, iodine and Astatine- general properties, oxidizing power, hydrogen halides, ionic and molecular halides, bridging halides, halogen oxides, oxoacids, interhalogen compounds, polyhalides, pseudohalogens and pseudohalides.

Sumon Chantwarly Mender (Industry Side







### Suggested texts and References:

(1) J. E. Huheey, 'Inorganic Chemistry - Principles of Structure and Reactivity' Harper & Row, 1988.

(2) F. A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', John Wiley, 1995.

(3) D. F. Shriver, P.W. Atkins and C.H. Langford, 'Inorganic Chemistry', OxfordUniversity Press, 1991.

(4) F. A.Cotton and G. Wilkinson, Basic Inorganic Chemistry, Wiley Easter, 1978.

(5) J. D. Lee, Concise Inorganic Chemistry, Van Nostrand Reinhold, 1977.

### CL 301: Chemistry Laboratory

Experiments of inorganic chemistry: Synthesis of coordination complexes, gravimetric analysis.

- 1. Preparation of Tetraamine Cupric Sulphate
- 2. Preparation of Potash alum
- 3. Preparation of Mohr's salt
- 4. Preparation of Epsom salt from Magnesium chloride
- 5. Preparation of Potassium trioxalate chromate (III)
- 6. Preparation of Nickel Ammonium Sulphate using Nickel Sulphate and Ammonium Sulphate
- 7. Preparation of Sodium trioxalato ferrate from ferric chloride, oxalic acid and sodium hydroxide
- 8. Preparation of Ammonium Ferric Sulphate using Ferrous Sulphate and Ammonium Sulphate
- 9. Preparation of Hexammine nickel (II) chloride
- 10. Preparation of Potassium Chlorochromate
- 11. Preparation of Cis-Potassiumdioxalatodiaquachromate
- 12. Preparation of Lead chromate
- 13. Preparation of Chrome alum
- 14. Preparation of Hexamine Cobalt (III) Chloride
- 15. Estimation of barium as barium sulphate in the given solution of barium chloride gravimetrically
- 16. Estimation of barium as barium sulphate gravimetrically and estimation of zinc volumetrically from the mixture of barium chloride and zinc oxide



Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
PCB401	Chemical Kinetics	[3+1]	4
CB401	Introductory Spectroscopy (UV-vis, fluorescence, IR, Raman, NMR)	[3+1]	4
C401	Properties of Matter	[3+1]	4
C402	Group theory	[3+1]	4
G401	Statistical Techniques and Applications	[2+0]	2
		Lab hrs	Credits
CL401	Chemistry Laboratory	[6]	3
GL401	Computational Laboratory and Numerical Methods	[4]	2
H401	Communication Skills Lab	[4]	2
	(100 of 240 credits)	Total	25
		25	

# **SEMESTER –IV**

(100 of 240 credits)

### PCB 401: Chemical Kinetics

#### UNIT-I:

**Basic Concepts:** Rate, order and molecularity of a reaction, Specific rate and specific rate constant, First, second and third order reactions – effect of concentration on reaction rate, rate expressions and integrated form, pseudo-unimolecular, nth order reaction of a single component.

### **UNIT-II:**

**Kinetic Measurements:** Experimental determination of reaction rates and order of reactions, Integrated rate method, Vant Haff differential rate method, Graphical method, Half life method, Ostwald dilution law method, initial rate as a function of initial concentrations. Order of complex reaction, Steady State approximation method, Equilibrium method, relaxation methods for fast reaction

### Unit-III:

**Factors Affecting Reaction Rate:** Effect of temperature on reaction rate – Arrhenius equation and activation energy, temperature coefficient theory, overall rate constant, overall activation energy, overall pre-exponential factor, effect of ionic strength on reactions between ions, kinetic salt effect, effect of solvent on ionic reaction, dielectric constant



### Unit-IV:

**Complex Reactions:** Kinetics of parallel first order reaction, Wegscheider Test, kinetics of reversible reaction/opposing reaction, kinetics of consecutive reaction, kinetics of photochemical reaction, radioactive decay, complex mechanisms involving equilibria.

#### Unit-V:

**Catalysis:** Homogeneous catalysis, basis of catalytic action, catalysis and the equilibrium constant, Michaelis-Menten kinetics, acid base catalysis, the Bronsted catalysis law, negative catalysis and inhibition, heterogeneous catalysis, surface reactions – effect of temperature and nature of surface

#### Suggested texts and References:

(i) K.A. Connors, Chemical Kinetics: A Study of Reaction Rates in Solution, V.C.H. Publications 1990. (ii)J.I. Steinfeld, J.S. Francisco and W.L. Hase, Chemical Kinetics and Dynamics, Prentice Hall 1989. (iii) Paul L. Houston, Chemical Kinetics and reaction dynamics.
(iv) K.J.Laidler, Chemical Kinetics, 3rd ed. Harper and Row, 1987.
(v) J.W. Moore and R.G. Pearson, Kinetics and Mechanisms, John Wiley and Sons, 1981
(vi) A. A. Forst and R. G. Pearson, Kinetics and Mechanism, Wiley International Edition.
(vii) Sanjay K. Upadhay, Chemical kinetics and Reaction Dynamics, Springer, 2006
(viii) Puri, Sharma, Pathania, Principles of Physical Chemistry

### **CB401: Introductory Spectroscopy**

(45 + 15 = 60 hrs)

### UNIT-I

(i) **The electromagnetic spectrum:** Nature of electromagnetic radiation. The electromagnetic spectrum and its regions. Absorption of electromagnetic radiation. Frequency, wavenumber, wavelength, Intensity: units and conversions. Boltzmann distribution.

(ii) **Spectroscopic Processes:** Absorption, emission, and scattering of light, reflection, refraction, diffraction, dispersion.

### UNIT-II

(iii) UV-VIS Absorption Spectroscopy: Principles and instrumentation of spectrophotometers. UV-Visible spectroscopy to determine conjugation. UV-visible spectroscopy and electronic transitions. Electronic ground states and excited states in organic molecules: n to pi-star and pi to pi-star transitions. band position and band intensities.

(iv) Fluorescence Spectroscopy: Principles and instrumentation of fluorimeters. Advantage of fluorimetry compared to absorption spectrophotometry. Luminescence and the fate of excited states: timescale of fluorescence and phosphorescence. Qualitative and Quantitative Fluorimetry.



### UNIT-III

(v) **IR** - Principles and instrumentation of Infrared spectroscopy. Infrared spectroscopy and molecular vibrational transitions. Simple dispersive IR spectrometer and ovewrview of modern instrumentation. Transmittance and absorbance. Vibrational modes and selection rules. Factors governing the position and intensity of IR bands: effects of variation in reduced mass and force constant. Group frequency and fingerprint regions: use of IR for identification by presence/absence of absorptions characteristic of specific bonds/bond groupings. Interpretationof IR spectra.

(vi) Raman Spectroscopy: Raman Effect and molecular polarizability. Technique and instrumentation. Pure rotational Raman spectra, vibrational Rama spectra. Structure determination from Raman and IR.

### **UNIT-IV**

(vii) Nuclear Magnetic Resonance (NMR): Introduction to Nuclear Magnetic Resonance (NMR) spectroscopy. 1H and 13C NMR, number of signals, integration, chemical shift, splitting of signals. Principles and instrumentation of NMR spectroscopy. Nuclear spin and nuclear magnetism. Energies of nuclear spin states in a magnetic field. Boltzmann population of nuclear spin states and the origin of NMR signals. Applications: Interpretation of simple 1H NMR spectra. Information from: chemical shifts and delta values, peak areas and integration, splitting patterns and spin-spin coupling constants. (n+1) rule and Pascal's triangle. Interpretation of NMR spectra using examples of organic compounds.

#### UNIT-V

(viii) Mass spectrometry: Introduction to mass spectroscopy (molecular mass, accurate mass and isotopes) Principles, ionisation methods (including EI, MALDI, ESI). Molecular ions and fragmentation processes under EI. Mass spectrometry for determining the molecular weight/formula of organic compounds and identify the presence of isotopes.

### C 401: Properties of Matter

#### (45 + 15 = 60 hrs.)

#### UNIT-I

(i) Gaseous State a). Perfect gases and gas laws, law of partial pressures and partial volumes, Graham's law of effusion, critical state and determination of the critical constants, continuity of state

(b) The kinetic theory of gases, pressure and temperature of a gas, derivation of the gas laws from the kinetic theory, The Boltzmann constant, Maxwell's law of distribution of molecular velocities,(c) Ideal and real gases, deviations of the real gases from the ideal gas laws, collision diameter, van der Waals equation, reduced equation of state, equation of state,

### UNIT-II

(ii) The Liquid State: (a) Vapour pressure, determination of vapour pressure, external and internal pressure, boiling point and vapour pressure.



(b) Surface tension, measurement of surface tension. Surface tension and vapour pressure, surface tension and temperature – Eootvos-Ramsay-Shields relation, parachor.

(c) Viscosity, measurement of relative and absolute viscosity, viscosity and temperature, molecular weight from viscosity.

### UNIT-III

(iii) The Solid State: (a) Crystalline and amorphous solids, Crystals – Steno's law, Hauy's law, Laws of symmetry. Crystals systems and lattices, Crystals and X-rays, Bragg's method of crystal analysis, Different kinds of crystal structures, methods of crystal analysis, electron diffraction, , magnetic properties - diamagnetic and paramagnetic materials. Ionic, covalent, metallic and coordinate bonds

(b) Radius ratio rules and coordination number, close packing. Classification of ionic structures – AX, AX2 and AX3 groups. Lattice Energy, Stoichiometric defects – Schottky and Frenkel. Non-stoichiometric defects – metal excess and metal deficiency.

#### UNIT-IV

(iv) Colloids: The colloidal system, preparation of colloidal systems, classification. Lyophobic sols - optical and electrical properties, effect of addition of electrolytes and applied electric field. Determination of zeta potential by electrophoresis and electroosmotic methods. Origin of charge and the mechanism of flocculation – stability of sols. Properties of Lyophilic sols – viscosity and protective action.

#### UNIT-V

Kinetic properties of sols and Brownian motion. Macromolecules – viscosity and molecular weight of polymers, osmotic pressure, The Donnan equilibrium. Sedimentation and ultracentrifuge, scattering of light. Protein sols, association colloids and emulsions

#### Suggested texts and References:

(1) P.W. Atkins, Physical Chemistry, Oxford University Press, 7th Edition, 2006.

(2) G.M. Barrow, Physical Chemistry, 5th Edition, Tata McGraw-Hill, New Delhi, 1992.

(3) D.A. McQuarrie and J.D. Simon, Physical Chemistry - a molecular approach, Viva Books Pvt.Ltd. (1998).

(4) D.K. Chakrabarty, Adsorption and catalysis by solids, Wiley Eastern, 1990.

(5) F.P. Kane and G.B. Larrabee (Eds.), Characterisation of solid surfaces, Plenum, 1978.

(6) A.W. Adamson, Physical Chemistry of Surfaces, 3rd Edn., Wiley Interscience, 1976.







### C 402: Group theory

### UNIT-I

(i) Symmetry Elements and Operations, Pure Rotations (CnRotations), Improper Rotations, Rotation-Reflection (Sn) & Rotation-Inversion (n-bar) Axes.

### UNIT-II

(ii) Point Groups: Low Symmetry Point Groups (C1, Ci, Cs), Simple Axial Point groups (c., S4n, Cnv' Cnh), Dihedral Groups (Dn, , Dnd, Dnh)

### UNIT-III

Platonic Solids & the "Cubic" Groups (Td, Oh , Ih ), Derived High Symmetry Groups (T, Th , 0, I), The "Infinite Groups" ( $C\infty v$  and  $D\infty h$ ), Points Groups & Chirality, Point Groups & Dipole Moment.

### UNIT-IV

(iii) Multiplication Tables (i.e., operation 1 followed by operation 2) for point groups. Similarity Transforms, Classes of Symmetry Elements. Naming Representations (Mulliken Symbols), Subgroups and Supergroups., Non-Commutative Operations.

### UNIT-V

(iv) Representations of Groups., Irreducible Representations., Character Tables. Their derivations and use of their contents. Matrix Representation of Symmetry Operations. The "Full Form" of the Character Table.

### Suggested texts and References:

1. F. A. Cotton, "Chemical Applications of Group Theory", 3rd Edition, John Wiley (1990). G 401: statistical techniques and its applications

### CL 401: Chemistry Laboratory

- 1. Preparation of acetyl salicylic acid (*aspirin*) from salicylic acid.
- 2. Preparation of Benzenalide from Aniline (Schotten-Baumann reaction).
- 3. Synthesis and characterization of Gold nanoparticle. Study on effect of various conc. of NaCl in aggregation of AuNPs.
- 4. Synthesis and characterization of Silver nanoparticle. Study on effect of various conc. of NaCl in aggregation of AgNPs.
- 5. Study on hydrolysis of ethyl acetate catalysed by 1M of HCl at room temperature and also study on effect of anionic surfactant SDS (sodium dodecyl sulphate)
- 6. Study on the rate of reaction of ethyl acetate at two different concentration of acid.
- 7. Study on the decomposition of  $H_2O_2$  by  $Fe^{3+}$  and  $Cu^{2+}$  at 35°C.









# <u>3rd Year</u>

# **SEMESTER –V**

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
CB501	Analytical Chemistry	[3+1]	4
C501	Quantum Chemistry	[3+2]	5
C502	Inorganic Chemistry II	[3+1]	4
C503	Organic Chemistry II	[3+2]	5
H501	Scientific Writing in Hindi	[2]	2
		Lab contact hrs	Credits
CL501	Chemistry Laboratory	[10]	5
	(124 of 240 credits)	Total	25

(125 of 240 credits)

#### **CB 501 : Analytical Chemistry**

(45 + 15 = 60 hrs.)

### UNIT-I

(i) Error analysis: Methods of sampling and associated errors, Classification of errors, Propagation of errors, treatment of errors, Normal distribution, Tests of Significance and Confidence Limits.

### UNIT-II

(ii) Separation techniques: Solvent Extraction Technique: Conventional, Liquid Membranes – Bulk, Supported and Emulsified, Solid Phase Extraction (SPE). Ion Exchange: Conventional, Membranes. Chromatography: Gas chromatography (GC), High Performance Liquid Chromatography (HPLC), Ion chromatography (IC).

### UNIT-III

(iii) Mass Spectrometry: Mass Analysers – Magnetic, Quadrupole, Time of Flight (TOF), Features – Resolution, Dispersion, Abundance, Sensitivity, Detectors, Ion Sources – Thermal Ionisation (TI), Electron Impact, ICP, GD, Laser Ablation (LA-ICP), Secondary Ionisation (SI), Matrix Assisted Laser Desorption and Ionisation (MALDI), Hyphenated Technique – IC-MS, HPLC-MS, GC-MS.

### UNIT-IV

(iv)Thermal Methods: Thermogravimetric Analysis (TGA), Derivative Thermogravimetric Analysis (DTG), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Evolved Gas Analysis (EGA).





(v)Electrochemical Methods: Introduction, Potentiometry, Ion Selective Electrodes (ISE), Voltammetry & Polarography, Cyclic, Pulse and Stripping Voltammetry, Coulometry and Amperometry, AC Electrochemical Techniques, Scanning Electrochemical Microscopy.

(vi) Detectors- Photomultiplier Tube (PMT), Charge Coupled Device (CCD), Charge Injection Device (CID), Spectrometers – Czerny Turner, Echelle, Sample Introduction Devices – Flame, Electrothermal, Laser Ablation, Direct Sample Insertion Devices, Interferences, detection limits, sensitivity.

### UNIT-V

(vii) Conductance of solutions and electrochemistry: Faraday's laws of electrolysis, Electrolytic conduction- Arrhenius theory of electrolytic dissociation, strong and weak electrolytes. Migration of ions – transference numbers, Determination of transference number using Hittrof's rule and moving boundary method. Conductance of solutions – electrolytic conductance, determination of conductance, equivalent conductance and concentration, Kohlrausch's law of independent migration of ions, ionic mobilities, temperature dependence. Hydration of ions, the interionic attraction theory. Applications of conductance measurements– degree of dissociation of weak electrolytes, dissociation constants of weak acids, degree of dissociation of water, basicity of organic acids, determination of solubilities of sparingly soluble salts, conductometric titrations, activities of electrolytic solutions, ionic strength. The Debye-Huckel theory of dilute ionic solutions.

#### Suggested texts and References:

(1) D.A. Skoog, D. M. West, F. J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edition, Thomson (2004).

(2) A.I. Vogel, A text book of Quantitative Analysis, 5th Edition Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, ELBS (1989).

(3) A. K. De, S. M. Khopkar and R. A. Chalmers, Solvent Extraction of Metals, Van Nostrand, Reinhold (1970).

(4) L. R. Snyder and J. J. Kirkland, Introduction to Modern Liquid Chromatography, 2nd Edition, Wiley (1979).

(5)Jose A. C. Broekaert, Analytical Atomic Spectrometry with flames and Plasmas, Wiley-VCH (2002).

(6) John Roboz, Introduction to Mass Spectrometry: Instrumentation and Techniques, Interscience (1968).



### C 501: Quantum Chemistry

(45 + 15 = 60 hrs.)

### UNIT-I

- (i) Foundations of quantum mechanics.
- (ii) Operator concept in quantum chemistry

### UNIT-II

(iii). Wave function for a free particle, the Schrodinger equation, physical interpretation of the Schrodinger equation wave function, Wave packets and the uncertainty principle,

(iv) Solution of Schrodinger's equation in some simple systems: one and three dimensional boxes, electron in a ring, rigid rotator, concept of tunnelling, one dimensional harmonic oscillator, hydrogen-like atoms, shapes of atomic orbitals.

### UNIT-III

(v) Approximate methods of quantum chemistry: perturbation and variation method, Timeindependent perturbation theory, Many electron systems: Orbital approximation, Slater determinant, Hartree-Fock self-consistent field theory. Slater type orbitals.

### UNIT-IV

Concept of LCAO, Huckel Theory, Huckel MOT, Angular momentum of many-particle systems, Born-Oppenheimer approximation, MO and VB theories illustrated with H<sub>2</sub>-molecule,

### UNIT-V

(vi)Spin orbital interaction; LS and JJ coupling. Spectroscopic term symbols for atoms. Molecules and Chemical bonding, Spectroscopic term symbols for diatomics; Directed valence & hybridization in simple polyatomic molecules.

#### Suggested texts and References:

(1) Ira N. Levine, Quantum ChemistryPrentice Hall India.

(2) John L. Powell and Bernd Crasemann, Quantum Mechanics, Oxford & IBH Publishing.

(3) A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw-Hill Publishing Comp. Ltd.

(4) David B. Beard, Quantum Mechanics, Allyn & Bacon, Inc, Boston.

#### C 502: Inorganic Chemistry II: UNIT-I

#### (45 + 15 = 60 hrs.)

### **Chemistry of d-block elements**

(i) General introduction to transition elements – Electronic structure, Metallic character, variable oxidation state, complexes, magnetic and catalytic properties.

### UNIT-II

(ii) Elements of the first transition series: Occurance, separation, extraction and chemistry of the scandium group (IIIB), titanium Group (IVB), vanadium group (VB), chromium group



(VIB), Manganeese group (VIIB).

### UNIT-III

Iron group (VIIIB(8)), Nickel group (VIII(9)) and Copper group (VIIIB(10)).

(iii) Chemistry of the elements of the second and third transition elements: fnium group (Group IVB), Niobium and Tantalum (Group VB), Molybdenum and tungsten (Group VIB); Technitium and Rhenium (Group VIIB),

### UNIT-IV

The Platinum group Metals, Ruthenium and Osmium (Group VIII(8)); Rhodium and Irridium (Group VIII(9)), Palladium and Platinum (Group VIII(10), Silver and gold Group (1B(11)).

### UNIT-V

### (iv)Chemistry of f-block elements-The lanthanide and actinide elements.

### Suggested texts and References:

- (1) Advanced Inorganic Chemistry, F. Albert Cotton and G. Wilkinson@1988, John Wiley & Sons.
- (2) J. D. Lee, Concise Inorganic Chemistry, Van Nostrand Reinhold, 1977.
- (3) J. E. Huheey, 'Inorganic Chemistry Principles of Structure and Reactivity' Harper & Row, 1988.

#### C 503: Organic Chemistry – II UNIT-I

(45 + 15 = 60 Hrs.)

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Prof. K. K. Ghosh Prof. Manas Kanti Deb

(A) Stereochemistry of Organic Compounds 25h (i) Isomerism – Concept and types (ii) Chirality: Configuration, stereogenic/chiral center, chirality and enantiomerism. Representation of configuration by flying wedge formulae and Fischer, Newman and Sawhorse projectionformulae. (iii) Stereochemistry of carbon compounds with upto three similar and dissimilar asymmetric carbon atoms; enantiomers, diastereomers, and racemic mixtures and their properties, resolution (chemical and chromatographic).

### UNIT-II

(iv) Diastereomerism: Threo, erythro, meso diastereomers. Geometrical isomerism in olefins, cycloalkanes and oximes. Absolute configuration: Assigning of stereochemical descriptors - R/S to Fischer projection and flying wedge formulae of chiral molecules and E/Z to olefins.

### UNIT-III

(v) Molecular chirality and elements of symmetry: Stereochemistry and stereochemical nomenclature of biphenyls, spirans, cummulenes, and alkylidene cycloalkanes (vi)Conformational concepts, conformations of acyclic molecules (ethane and butane), cyclohexane and mono, disubstituted cyclohexanes. Conformationally rigid and mobile diastereomers. (vii) Stereoselectivity and stereospecificity of organic reactions: Enantiomeric and diastereomeric selectivities.

### UNIT-IV

Prof. Guton Kunna Patra

shalk Basha External member (Acodemics)

The mechanism and stereochemical outcome of the following reactions: (a) SN1, SN2 and SNi reactions (b) Catalytic hydrogenation of alkenes (c) Ionic trans addition of bromine to alkenes (d) Epoxidation of alkenes, acid catalysed ring opening of epoxides. (e) Reactions of OsO4 and

Sumon Chantworly Menter (Industry Side) Ar. Allepa Pauly Chok



KMnO<sub>4</sub> with olefins (f) E2 reactions. (g) Topocity and prostereoisomerism - Enantiotopic and diastereotopic atoms, groups and faces.

### UNIT-V

**Chemistry of Alicyclic compounds:** Cycloalkanes and cycloalkenes. Factors affecting stability of conformations, conformation of cycloalkanes. Reaction mechanism in alicyclic compound. Conformation of Cyclic System: Monocyclic compounds and Fused ring and Bridged ring

Compound. Chemistry of Carbon radical (Single electron transfer mechanism): neighboringgroup participation; non-classical carbocataion; S<sub>Ni</sub> mechanism. Rearrangements of Carbocataion, Free-radical: Allylic, Pinacol/ Pinacolone, 1,2 rearrangements etc and rearrangement to heteroatoms. Pericyclic reaction and FMO approach.

### Suggested texts and References:

(1) I. L. Finar, Organic Chemistry, Vol. 1 & 2, ELBS.

(2) R. K. Bansal, Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, Wiley Eastern Ltd., 1990.

(3) J.A.J. Joule and G.F. Smith, Heterocyclic Chemistry, ELBS, 2nd Ed., 1982.F.G. Riddell, The Conformational Analyis of Heterocyclic Compounds, Academic Press, 1980.

(4) L.A. Paquette, Principles of Modern Heterocyclic Chemistry, W.B. Benjamin, Inc., 1978.(5) B.M. Acheson, An Introduction to the Chemistry of Heterocyclic Compounds, Interscience, 2nd Ed., 1975.

### CL 501 Chemistry Laboratory:

**1.** Determination of concentration of  $K^+$  ion in given water sample by using flame photometer.

**2.** Conductometric study of Saponification of ethyl acetate by sodium hydroxide at equal concentration of ester and alkali at room temperature.

**3.** Determine of concentration of Na<sup>+</sup> ion in given water sample by using flame photometer.

**4.** Conductometric study of Saponification of ethyl acetate by potassium hydroxide at equal concentration of ester and alkali at room tempreture.

**5.** Determination of the concentration of Fe in a sample of water using ammonium thiocyanate by spectrophotometer.

**6.** Determination of the concentration of Fe in a sample of water using 1,10\_phenanthroline by spectrophotometer.

**7.** Determination of strength of given HCl solution by titrating it potentiometrically against a solution of sodium hydroxide.

**8.** Isolation of lycopene from tomatoes.

**9.** Isolation of caffeine from tea leaves.

**10.** Isolation of casein and lactose from milk.

**11.** Isolation of piperine from black paper.



<b>SEMESTER -VI</b>
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Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
CB601	Biophysical Chemistry	[3+1]	4
C601	Atomic and molecular spectroscopy	[2+1]	3
C602	Inorganic Chemistry III	[2+1]	3
C603	Organic Chemistry III	[3+1]	4
C604	Nuclear Chemistry	[3+1]	4
H601	Ethics in Science and IPR	[2+0]	2
H602	Scientific Writing in English	[2]	2
		Lab contact hrs	Credits
CL601	Chemistry Laboratory	[6]	3
		Total	25

#### (150 of 240 credits)

### **CB 601: Biophysical Chemistry**

### UNIT-I

(i) The Chemistry of Life: An introduction: Physical properties of water: Structure, water as solvent, The hydrophobic effect, osmosis and diffusion. Introduction to Biomolecules: Nucleic Acid, Protein - Polymer Description of Macromolecular Structure, Intermolecular and Intramolecular forces, Non Covalent Interaction

### UNIT-II

(iii) **General principles of Biophysical chemistry I:** Hydrodynamic properties: Diffusion and sedimentation, determination of molecular weight from sedimentation and diffusion; Introduction of Ultra Centrifugation, Dynamic Light Scattering and Electrophoresis. Spectroscopic properties of proteins and nucleic acid: UV/Vis, Intrinsic fluorescence, Circular dichroism.

### UNIT-III

(iii) General principles of Biophysical chemistry II: The concept and application of Chemical and Physical equilibria in Biological system, The equilibrium constant and Standard Gibbs Free energies of reactants and products, Temperature dependence of the equilibrium constant, Double Strand formation in nucleic acid, Ligand-protein binding, Protein denaturation and stability, Introduction of DSC and ITC.

### UNIT-IV

(iv) Molecular self-assembly and Molecular medicine: Protein folding kinetics and Biophysical methods, Misfolding and aggregation; Physical basis of conformation diseases, Therapeutic approaches to protein misfolding diseases.



### UNIT-V

(v) Introduction to basic principles of protein X-ray crystallography, NMR, Small Angle X-ray scattering (SAXS), and Electron microscopy (EM).

### Suggested texts and References:

(1) Tinoco, Sauer, Wang, and Puglisi. (2003) Physical Chemistry: Principles and Applications in the Biological Sciences. Prentice Hall, Inc.

(2) Physical Chemistry for the Life Sciences: Peter Atkins and Julio de Paula(3) General review papers Dobson CM. Principles of protein folding, misfolding and aggregation. Semin Cell Dev Biol. 2004 Feb;15(1):3-16.

#### C 601: Atomic and molecular Spectroscopy

(45 + 15 = 60 hrs.)

### UNIT-I

(i) Born-Oppenheimer approximation - rotational, vibrational and electronic energy levels of homonuclear and heteronuclear diatomic and polyatomic molecules.

### UNIT-II

(ii) Microwave Spectroscopy: Rotational of molecules and rotational spectroscopy of rigid diatomic molecules, Effect of isotopic substitution, The non-rigid rotator and rotational spectra. Rotational spectra of polyatomic molecules – linear, symmetruic top and asymmetric top. Techniques and instrumentation.

### UNIT-III

(iv) Infrared spectroscopy: energy levels of vibrating diatomic molecule, simple harmonic oscillator and anharmonic oscillator, diatomic vibrating rotator, vibration-rotation spectra of CO. Breakdown of B-O approximation – interaction of rotations and vibrations. Vibrations of polyatomic molecules – Fundamental vibrations and their symmetry, overtone and combination frequencies, influence of rotation on the spectra of polyatomic molecules – linear and symmetric top molecules. Influence of nuclear spin. Group frequencies andanalysis of spectra, Techniques and instrumentation, FTIR spectroscopy

### UNIT-IV

(iv) Raman Spectroscopy: Classical and quantum theories of Raman effect and molecular polarizability. Pure rotational Raman spectra, Vibrational Raman spectra, Polarization of light and the Raman effect, Structure determination from Raman and infrared spectroscopy, Techniques and Instrumentation, Near IR FT Raman spectroscopy. Resonance Raman and electronic Raman transition and applications.

### UNIT-V

(v) Electronic spectroscopy – Electronic structure and spectra of diatomic and polyatomic molecules. Techniques and instrumentation, Molecular photoelectron spectroscopy

(vi) Electron spin resonance spectroscopy- spin and spectra, relaxation processes, origin of g-factor and hyperfine coupling, Kramer's degeneracy, ESR of transition metal complexes,



### Application of ESR Spectra

#### Suggested texts and References:

(1) G. M. Barrow, Molecular spectroscopy

(2) C.N. Banwell and E. M. McCash, Fundamentals of Molecular spectroscopy, Tata McGraw HillPub. Co.New delhi

(3) J. D. Graybeal, Molecular Spectroscopy, McGraw Hill International Book Co. N.Y.

(4) Puri, Sharma, Pathania, Principles of Physical Chemistry

### C 602: Inorganic Chemistry III

(45 + 15 = 60 Hrs.)

#### UNIT-I

(i) Coordination compounds, Werners's theory, effective atomic number, coordination number, shapes of d-orbitals and bonding in transition metal complexes, stability of complexes, the chelates and macrocyclic effects, types of classification of ligands, second sphere of coordination,  $\pi$ -complexes,  $\pi$ -acid ligands, multiple bonds from ligands to metals. **UNIT-II** 

(ii) Crystal Field theory – crystal filed splitting and elementary treatment of the electronic spectra, Jahn-Teller distortion of octahedral complexes, square planar complexes, tetrahedral complexes, magnetic properties of 3d compounds.

#### UNIT-III

(iii) MO theory, Nomenclature of coordination compounds, d-orbital splitting in various fields -Spectroscopic states ,Tanabe-Sugano and Orgel diagrams , Derivation of Ligand field parameters (Dq. B) from electronic spectra, Magnetic moments , Orbital contribution, spin-orbit coupling and covalency.

### UNIT-IV

Molecular orbitals and energy level diagrams for common symmetries.

(iv) Bonding involving-donor ligands, Back-bonding, f-orbital splitting, Spectral and magnetic properties of f-block elements.

#### UNIT-V

(v) Reaction mechanisms: Substitution reactions - Dissociative and associative interchange - trans-effect - Linear free energy relations. Rearrangements - Berry pseudo rotation, Electron transfer reactions. Photo-dissociation, substitution and redox reactions, Fluxional molecules.



#### Suggested texts and References:

(1) F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley Eastern, John Wiley, 6th Ed., 1999.

(2) J.E. Huheey, E. Keiter and R. Keiter, Inorganic Chemistry, 4th Ed., Harper Collins College Publisher, 1993.

(3) D.Banerjea, Inorganic Chemistry Principles, Books Syndicate Pvt. Ltd., 2000.

(4) N.N. Greenwood and E.A. Earnshaw, Chemistry of Elements, Pergamon Press, 1989.

(5) J.J. Kratz, G.T. Seaborg and L.R. Morss; *The Chemistry of Actinide Elements*, 2nd Edition, Vol. 1&2, Chapman & Hall, New York (1986).

(6) J.C. Bailar, H.J. Emelius, R. Nyholm and A.F. Trotman-Dickenson; Comprehensive

#### C 603: Organic chemistry III

#### (45 + 15 = 60 Hrs.)

#### UNIT-I

Chemistry of Natural Products:

(i) **Terpenoids:** Classification, structure, chemistry and biogenesis of some important mono; sesqui,di, and triter penes.

#### UNIT-II

(ii) Steroids: Sterols and bile acids, estrogens, androgens, gestogens and adrenocortical hormones. Hormone production. Cardiac glycosides. Steroidal triterpenes; biogenesis of steroids and correlation with terpenoids.

### UNIT-III

(iii) Alkaloids: Characteristic reactions, general methods of degradation, structure and chemistry of some well-known alkaloids.

### **UNIT-IV**

(iv) Natural Pigments: anthocyanines, Flavones, flavanones, isoflavones, xanthones, quinones, pterins, chlorophyll and haemin.

### UNIT-V

(v) Carbohydrates: Stereochemistry, reaction and conformation of monosaccharides, deoxy and aminosugars, hexonic acid and vitamin C, disaccharides, polysaccharides, inositol; gan- gliosides and other glycosides. Chemistry of vitamins A, B, C and E.

#### Suggested texts and References:

- (1) I. L. Finar, Organic Chemistry, Vol. 1 & 2, ELBS.
- (2) J. Singh, S. M. Ali, J. Singh, Natural Products Chemistry.



### C 604: Nuclear Chemistry

### UNIT-I

(i) Nuclear Stability: Concept of nucleus and properties, nuclear mass and binding energy, elemental abundance, radioactive decay laws and equilibria. Nuclear Models: Liquid drop model, Shell model, Fermi gas model, collective model, optical model, concept of spin, parity electric and magnetic moments, isomerism.

### UNIT-II

(ii) Modes of Decay:  $\alpha$  decay,  $\beta$  decay, electron captures, de-excitation, internal conversion, artificial radioactivity.

(iii) Nuclear reactions: Energetics, cross-section, centre of mass system, angular momentum, compound nucleus, statistical model, nuclear fission and fusion, nuclear reactors, Heavy ion induced reactions, Accelerators.

### UNIT-III

(iv) Applications of radioactivity: preparation of radioisotopes, Szilard-Chamers' reaction, Concept of tracers, chemical yield, radiochemical purity, Application of radiotracers in Chemical Sciences, uses of nuclear radiations, radioisotopes as a source of electricity.

### UNIT-IV

(v) Elements of Radiation Chemistry: Interaction of radiation with matter, radiation dosimetry, radiolysis of water and some aqueous solutions, other radiolytic events.

(vi) Nuclear Methods: Activation Analysis – Neutron Activation Analysis (NAA),

Charged Particle Activation Analysis (CPAA), X-ray fluorescence (XRF) spectrometry,

### UNIT-V

Ion Beam Analysis – Backscattering Spectrometry (BS), Particle Induced Υ-ray Emission (PIGE), Nuclear Reaction Analysis (NRA), Elastic Recoil Detection Analysis (ERDA), Particle Induced X-ray Emission (PIXE).

### Suggested texts and References:

(1) G. Friedlander, J. Kennedy, Nuclear and Radiochemistry (1981) –J. M. Miller and J. W. Macias

- (2) R. D. Evans, Atomic Nucleus (1955)
- (3) S. Glasstone, Source book of Atomic Energy (1969)
- (4) G. T. Seaborg, Man made elements (1963).
- (5) H. J. Arnikar, Essentials of Nuclear Chemistry (1982).
- (6) C. Keller, The Chemistry of Transuranium Elements (1971).
- (7) J.C. Bailar, H.J. Emelius, R. Nyholm and A.F. Trotman-Dickenson; Comprehensive Inorganic Chemistry, Vol. 5, Pergamon Press, Oxford (1973).



### H601: Ethics of Science and IPR

### Unit-I

Introduction to Ethics– causes of unethical acts, Definition – moral, values, ethics; Role and importance of ethics in science; Professional ethics – professional conduct, Teaching ethical values to scientists, good laboratory practices, good manufacturing practices, Basic Approaches to Ethics; Posthumanism and Anti-Posthumanism.

### Unit-2

Medical Ethics: Different themes pertaining to medical ethics including ethical issues in public health. Environmental Ethics, Bioethics, Journals and Publishers: Monopolistic practices by Academic Publishers. Plagiarism, softwares for plagiarism detection.

### Unit-3

Introduction to IPR; Types of Intellectual property – Patents, Trademarks, Copyrights and related rights; Traditional vs. Novelty; Importance of intellectual property rights in the modern global economic environment, Importance of intellectual property rights in India.

### Unit-4

Patents: Definition, patentable and non patentable inventions; types of patent application – Ordinary, Conventional, PCT, Divisional, and Patent of addition; Concept of Prior Art; Precautions while patenting disclosure / nondisclosure;

### Unit-5

Case studies and agreements - Evolution of GATT and WTO and IPR provisions under TRIPS; Madrid agreement; Hague agreement; WIPO treaties; Budapest treaty; Indian Patent Act (1970) **Suggested texts and References:** 

1	David B. Resnik	The Ethics of Science: An Introduction', Routledge, New York, 1998
2	V. K. Ahuja	Intellectual Property Rights in India', 2015
3	V. K. Ahuja	Law Relating to Intellectual Property Rights', 2017.

### CL 601: Chemistry laboratory:

**1.** To determine the total alkalinity in a given water sample.

**2.** To determine the CMC (Critical Micelle Concentration) of surfactant by fluorescence technique using pyrene as a probe.

3. Determination of Lead (Pb) in given water sample using Dithiozone by spectroscopically.

4. Determination of Molybdenum using Potassium Thiocynate by solvent extraction method.

**5.** To construct the phase diagram for three component system.



**6.** Synthesis of hexaammine cobalt(III) chloride,  $[Co(NH_3)_6Cl]^{3+}$ .

**7.** Synthesis of pentaammine cobalt(III) chloride.

**8.** Determination of the acid dissociation constant of methyl red using spectrophotometric method.

And some experiments based on analytical techniques such as cyclic voltammetry, pulse polarography, electrodeposition, gas chromatography, nuclear magnetic resonance, FTIR, thermal gravimetry methods, atmic absorption spectroscopy etc.



**FOURTH YEAR** 

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
C701	Photochemistry	[3+1]	4
C702	Chemical Biology	[3+1]	4
C703	Organometallics & Bio-inorganic Chemistry	[3+1]	4
C704	Physical Organic Chemistry	[3+1]	4
CPr701	Reading Project	-	4
		Lab contact hrs	Credits
CL701	Advanced Chemistry Laboratory-I	[10]	5
		Total	25

### (175 of 240 credits)

### **C701: Photochemistry**

### (45 + 15 = 60 hrs.)

#### UNIT-I

#### **Basic Principles of photochemistry:**

(i) **Photophysical processes:** Deexcitation processes for the excited molecules (fluorescence, phosphorescence, delayed emission, nonradiative relaxation, excimer and exciplex formation, heavy atom effect, etc.). Kinetics of excited state processes and quantum yields of different processes.

#### UNIT-II

(iii) Photoinduced processes: Photo-dissociation, photo-ionization, intramolecular charge and proton transfer processes, intermolecular electron and proton transfer reactions, intra and intermolecular energy transfer processes

(iv) Applications of photochemistry: Photosynthesis, vision, solar energy conversion, atmospheric photochemistry, etc.

### UNIT-III

(v) Organic Photochemistry Distinctive features of photochemical reactions, methods of preparative photochemistry, Photochemistry of alkenes, alkynes and related compounds – geometrical isomerism, electrocyclic processes, sigmatropic shifts, di- $\pi$  methane reactions, addition, cycloaddition and oxidative reactions.

### UNIT-IV

(vi) Photochemistry of aromatic compounds – bond cleavage and hydrogen abstraction reactions, cycloaddition reactions, rearrangements of cyclo-hexenones and cyclo-hexadienones, thiocarbonyl compounds. Photochemistry of other organic compounds – imines, imminium salts, nitriles and nitro compounds, azo and diazo compounds, diazonium salts, sulphur and halogenated



compounds, photohalogenation and photonitrosation reactions. Photooxidation of alkanes. photochemistry of carbonyl compounds.

### UNIT-V

(vii) **Inorganic Photochemistry** Introduction to inorganic photochemistry. Photophysical processes. The electronic absorption spectra of inorganic compounds. Characteristics of the electronically excited states of inorganic compounds. Photoelectochemistry of excited state redox reactions. Photosensitization. Photochemical reactions; substitution, decomposition and fragmentation, rearrangement, and redox reactions. Ligand field photochemistry of dncomplexes.

#### Suggested texts and References:

K.K.Rohatagi-Mukherjee, Fundamentals of Photochemistry, Wiley Eastern, 1978.
 M.S.Wrighton, Inorganic and Organometallic photochemistry, ACS Pub., 1978.
 V. Balzani and V. Carasiti, Photochemistry of Co-ordination compounds, Academic Press, 1970.

(4) J. D. Coyle, Introduction to Organic Photochemistry, ISBN

### C 702: Chemical Biology

#### (45 + 15 = 60 Hrs.)

### UNIT-I

(*i*) **Structure and the Synthesis of Life:** Central Dogma, Introduction to Biological Chemistry, Artificial gene synthesis: solid-phase DNA synthesis Versus molecular cloning and polymerase chain reaction (PCR). Synthia and Mycoplasma laboratorium,

### UNIT-II

DNA digital data storage, Peptide and protein synthesis. Lipid synthesis, Carbohydrate and membrane synthesis.

What Chemists Can Do for Biology: Natural Versus non Natural amino acid, Nonnatural Amino Acids for Site-Specific Protein Conjugation, Bio-orthogonal chemistry, Chemical genetics, reverse chemical genetics.

### UNIT-III

**Biomimetic Chemistry:** Compounds that mimics a biological material in its structure or function, Artificial Enzymes: Chemical transformation, Molecular recognition (Mimic binding), examples of mimics found in research and industry: Cyclodextrins Cryptands,

### **UNIT-IV**

Catalytic antibodies. Nanozymes- next-generation artificial enzymes, A laboratory procedure designed to imitate a natural chemical process: Biomimetic synthesis, Natural product synthesis, Asymmetric catalysis, Reaction methodology.

### UNIT-V

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(iv) Metabolomics: Technologies in metabolomics. Nutrigenomics. Other omics. Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry in metabolomics. Metabolic pathways resources: KEGG, Biocarta. Nutrigenomics and metabolic health. Solved problems and future



challenges.

### Suggested texts and References:

(1) G. Friedlander, J. Kennedy, Nuclear and Radiochemistry (1981) –J. M. Miller and J. W. Macias

(2) R. D. Evans, Atomic Nucleus (1955)

(3) S. Glasstone, Source book of Atomic Energy (1969)

(4) G. T. Seaborg, Man made elements (1963).

(5) H. J. Arnikar, Essentials of Nuclear Chemistry (1982).

(6) C. Keller, The Chemistry of Transuranium Elements (1971).

(7) J.C. Bailar, H.J. Emelius, R. Nyholm and A.F. Trotman-Dickenson; Comprehensive Inorganic Chemistry, Vol. 5, Pergamon Press, Oxford (1973).

### C703: Organometalics and Bioinorganic Chemistry (45 + 15 = 60 hrs.)

### UNIT-I

**Organometallics:** Overview, 18-electron rule, square planar complex. Carbonyl ligand – bonding, binary carbonyl complexes, oxygen-bonded carbonyls, other ligands similar to CO, IR spectrum, main group parallels with binary carbonyl. Pi-ligands – linear and cyclic pi systems, NMR spectra of organometallic complexes.

# UNIT-II

Structure and bonding of metal alkyls and aryls, complexes with  $\pi$ -acids, CO and relatedligands, complexes with olefins, acetylenes and related unsaturated molecules, catalytic properties of mononuclear compounds, boranes, carboranes and metallocarboranes, bimetallic and cluster complexes.

### UNIT-III

Complexes containing M – C, M = C, M = C bonds, hydride and dihydrogen complexes, phosphines and related ligands.

(ii) Organometallic reactions occurring in metal – ligand substitution, oxidative, addition, reductive, elimination. Organometallic reactions involving modification of ligands – insertion and deinsertion, nucleophilic addition to ligands, nucleophilic abstraction, electrophilic reactions.

# UNIT-IV

Homogeneous catalysis and heterogeneous catalysis – use of transition metal complexes, hydroformylation reaction, Walker-Smidt synthesis of acetaldehyde, hydrogenation, Monsanto acetic acid process. Transition metal carbine complexes – structure, preparation and chemistry, metathesis and polymerization reactions

# UNIT-V

(iii) **Bio-inorganic chemistry** - biochemistry of iron - its storage, transport and function, copper and zinc proteins, biological activation of oxygen, bioinorganic chemistry of alkali and alkaline earth metal cations, photosynthesis, nitrogen fixation, toxicity of metals. Chemistry aspects of metal complexes. Spectral, biochemical and biological methods used in bioinorganic chemistry. Bioinorganic chemistry of Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup> and Ca<sup>2+</sup>. Role of metal ions in biology : Proteins and



enzymes of V, Mn, Fe, Co, Ni, Cu, Zn and Mo. Structural and functional models. Transport and storage of metal ions. Carcinogenicity of chromium. Selenium in biology.

#### Suggested texts and References:

(1) G.O.Spessard, G.L.Miessler, Organometallic Chemistry, Prentice Hall, 1997.

(2) C.Elsehenbroich and A. Salzer, Organometallic Chemistry, 2nd Ed., Wiley VCH, 1992.

(3) F.A.Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley, 1999.

(4) N.N.Greenwood and A. Earnshaw, Chemistry of the Elements, lst Edn., Pergamon, 1985.

(5) S.J.Lippard & J.M.Berg, Principles of bioinorganic chemistry, University Science Books, Mill Valley, 1994.

(6) I. Bertini, H.B.Gray, S.J.Lippard and J.S.Valentime, Bioinorganic Chemistry, Univ. Sci. Books, Mill Valley, 1994.

(7) James A.Cowan, Inorganic Biochemistry, VCH Publishers, 1993.

#### C 704: Physical organic chemistry

(45 + 15 = 60 hrs)

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Prof. K. K. Ghosh Prof. Manas Kanti Deb

#### UNIT-I

**Structure and Models of Bonding:** Basic Bonding Concepts, Bonding and Structure of Reactive Intermediates, Molecular Orbital Theory, electron in a box problem, energies and coefficients of linear pi-systems, Secular Determinant, Huckel MOT, HMOT in cyclic andacyclic pi-systems, Aromatic and antiaromatic systems.

### UNIT-II

(ii) Strain and Stability: Thermochemistry of Stable Molecules, Thermochemistry of Reactive Intermediates, Relation Between Structure and Energetics-Basic Conformational Analysis, Conformations of Acyclic and Cyclic Systems, Electronic Effects.

Acid-Base Chemistry: Bronsted Acid-Base Chemistry, Aqueous and Non-Aqueous Systems, Predicting Acid Strength in Solution, Lewis Acids/Bases and Electrophiles/Nucleophiles.

### UNIT-III

(iv) Thermal Pericyclic Reactions: Cycloadditions, Orbital correlation diagram, Frontier Molecular Orbital, Comments on forbidden and allowed reactions, Photochemical pericyclic reactions, D-A cycloadditions, regio- and stereoselectivity, endo-effect, [2+2] cycloaddition, ketene cycloaddition, 1,3-dipolar cycloaddition, ene-reaction, retrocycloaddition, electrocyclic reactions, sigmatropic rearrangements, Claisen and Cope rearrangements, Cheletropic reactions.

### UNIT-IV

(v) Reactivity, Kinetics and Mechanisms: Energy Surfaces and Related Concepts, Postulates and Principles Related to Kinetic Analysis, Kinetic Experiments and Deciphering Mechanisms. (iv)Experiments Related to Thermodynamics and Kinetics: Isoptope Effects, Substituent Effects, Hammett Plots and Linear Free Energy Relationships, Other Linear Free Energy Relationship, Acid-Base Related Effects.

#### UNIT-V

- Reap Gutan Kunnas Patra

th Institute) External member (Academics)

(vii) Application of physical methods: Deciphering mechanisms of electrophilic and nucleophilic

Ar. Alepa Pauly Chit



substitution/additions, eliminations, cyclizations, radical reactions and reactions involving reactive intermediates.

### Suggested texts and References:

(1) E. V. Anslyn and D. A. Dougherty, Modern Organic Chemistry, University Science, 2005.

(2) I. Fleming, Molecular Orbitals and Organic Chemical Reactions, John Wiley, 2009.

(3) J. Clayden, S. Warren, N. Greeves, P. Wothers, Organic Chemistry, 1st Edition, Oxford University Press, 2000

(4) F. J. Carey and R. J. Sundburg, Advanced Organic Chemistry, Part A and Part B, 5th Ed., Springer, 2007

(5) J. March, Advanced Organic Chemistry, 3rd edition, McGraw Hill, 1991.

(6) S. H. Pine, Organic Chemistry, 5th edition, McGraw Hill, 1987.

# **CL-701 Chemistry Laboratory**

- 1. Green synthesis and characterization of silver nanoparticle (AgNPs) using leaf extract of basil (*Ocimum sanctum*).
- 2. Green synthesis and characterization of silver nanoparticle (AgNPs) using mango (*Magnifera indica*) leaf extract.
- 3. To synthesize and characterize the CdTe quantum dots using UV-VIS and Fluorescence. Also calculate the diameter (size), Band gap and FWHM (Full Wave Half Maxima) of quantum dot.
- 4. Determination of salinity of given water sample using conductivity meter.
- 5. Determination of solubility and solubility product of sparingly soluble salt (BaSO<sub>4</sub>) conductometrically.
- 6. To determine the distribution coefficient of iodine between CCl<sub>4</sub> and H<sub>2</sub>O at room temperature
- 7. To extract the essential oil of Eucalyptus citriodora leaves using Clevenger's apparatus
- 8. To extract the essential oil of ginger using Clevenger's apparatus
- 9. To extract the essential oil of *Ocimumtenuiflorum* (Tulsi) leaves using Clevenger's apparatus.
- 10. Determination of SO<sub>4</sub><sup>-2</sup> (sulphate) ion concentration in given water sample by nephloturbidity meter.
- 11. To Synthesize the Gold Nanoparticles using Tea Powder extracts.
- 12. To investigate the adsorption of acetic acid from aqueous solution by activated charcoal, verifying Freundlich and Langmuir adsorption isotherm.









# **SEMESTER –VIII**

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
C801	Chemistry of Materials	[3+1]	4
C802	Macro and Supra-molecular chemistry	[3+1]	4
C803	Reaction Dynamics	[3+1]	4
C804	Heterocyclic Chemistry	[3+1]	4
		Lab contact hrs	Credits
CL801	Advanced Chemistry Laboratory-II	[10]	5
CPr801	Project	-	4
		25	

(200 of 240 credits)



#### **C801:** Chemistry of Materials

#### UNIT-I

#### **Basic Aspects of the Solid State**

(i) Solid State Structure: Primitive lattice vectors - reciprocal lattice - crystal systems and desymmetrization schemes. Bravais lattices; closed packed structures, octahedral and tetrahedral holes, crystallographic point groups and space groups - organic and in organic crystal structure motifs - polytypes and polymorphs. pervskites and related structures, normal and inverse spinels.
(ii) Defects and Non-stoichiometry: Intrinsic and extrinsic defects - point, line and plane defects; vacancies, Schottky defects, Frenkal defects - Charge compensation in defective solids - non-stoichiometry, thermodynamic aspects and structural aspects. Miller and Weiss Indices.

#### UNIT-II

(iii) Thermal Properties: Free electron theory, electrical conductivity, Hall effect - band theory, band gap, metals and semiconductors - intrinsic and extrinsic semiconductors, hopping semiconductors - semi-conductor/metal transition - p-n junctions - superconduction, Meissner effects, type I and II superconductors, basic concepts of BCS theory, Josephson device (iv) Ionic Conductors: Types of ionic conductors, Mechanism of ionic conductors, examples and

(iv) Ionic Conductors: Types of ionic conductors, Mechanism of ionic conductors, examples and applications of ionic conductors.

#### UNIT-III

(v) High Tc Materials: Defect pervskites - high Tc superconductivity in cuprates – preparation and characterization, normal state properties, anisotropy, temperature dependence of electrical resistance, optical phonon modes – superconducting state, heat capacity, coherence length, elastic constants, positron lifetimes, microwave absorption - pairing and multigap structure in high Tc materials - applications of high Tc materials. Magnetic and optical properties of High Tcmaterials.

#### **UNIT-IV**

(viii) Synthesis of Materials: Phase diagrams - preparation of pure materials, mass transport, nucleation and crystal growth - preparative techniques, zone refining, chemical transport, etc. (ix) Multiphase materials: Ferrous alloys, Fe-C phase transformations in ferrous alloys, stainless steels - non-ferrous alloys - properties of ferrous and non-ferrous alloys and their applications.

(x) Thin Films, Langmuir-Blodgett Films: Preparation techniques, evaporation/sputtering, chemical processes, MOCVD, sol-gel etc., LB film growth techniques, photolithography, properties and applications of thin films

#### UNIT-V

(xi) Liquids Crystals: Mesmorphic behavior - thermotropic and lyotropic phases – description of ordering in liquid crystals, the director field and order parameters - nematic and semectic mesophases, smectic -nematic transition and clearing temperature - homeotropic, planar and twisted nematics - chiral nematics - smectic A and smectic C phases - cholesteric-nematic transition - optical properties of liquid crystals - effect of external field.



(xii) Organic Solids, Fullerenes, Molecular Devices: Conducting organics – organic superconductors - magnetism in organic materials.

(xiii) Nonlinear Optical Materials: Nonlinear optical effects, second and third order – molecular hyperpolarisability and second order electric susceptibility - materials for second and third harmonic generation.

#### Suggested texts and References:

(1) H.V. Keer, Principles of the Solid State, Wiley Eastern (1993).

(2) N.W. Ashcroft, N.W. Mermin, Solid State Physics, Saunders College, Philadelphia (1976).

(3) W.D. Callister, Material Science and Engineering. An Introduction, Wiley, New York (1985).(4) Charles Kittle, Introduction to solid state physics, John Wiley & Sons, New York (1968).

Anthony R.West, Solid State Chemistry and its Applications, John Wiley & Sons, New York (2005).

(5) Lesley E. Smart, Elaine A. Moore, Solid State Chemistry (3rd Ed), Taylor & Francis (2005).
(6) N.N. Greenwood, Ionic crystals, lattice defects and non-stoichiometry,

#### C 802: Macro and Supramolecular Chemistry

(45 + 15 = 60 hrs.)

#### UNIT-I

#### A. Polymer Chemistry

(i) Polymerization reactions, mechanism and kinetics – cationic, anionic and radical polymerization. Template, emulsion and electrochemical polymerization, Condensation, ring opening, step growth and radiation polymerization reactions. Coordination complex polymerization, Naturally occurring polymers, Biological polymers, inorganic polymers. Polymerization of cyclic organic compounds. Copolymerization and multicomponent polymerization,

(ii) Thermodynamics and kinetics. Polymerization and depolymerization equilibria - Kinetics of condensation (Step-Growth), Free radical and ionic polymerizations.

### UNIT-II

(iii) Physical Characterization: Fabrication and Testing, Relationship between structure and properties - Thermal, flame and chemical resistance - Additives - Electroactive polymers - Biomedical applications. Molecular wieght (Mn, Mw) determination - Morphology -Glass transitions and crystallinity, NMR and neutron scattering studies.

(iv) Reactions and degradation of polymers, biodegradable polymers. Thermal and oxidative degradation, catalysis by macromolecules, computer applications.

### UNIT-III

#### Supramolecular Chemistry

(i) Fundamental of supramolecular chemistry: Definitions, brief overview & examples, types of non-covalent interactions (H-bonding, electrostatic (ion-ion, ion-dipole, dipole-dipole) hydrophobic and steric,  $\pi$ - $\pi$ , vander waals), concepts of host guest complexation with examples, macrocyclic effect, complexation of neutral molecules, self-assembly, molecular boxes and capsules, self-complementary species and self-replication.



### **UNIT-IV**

(ii) The Most Interesting Macrocyclic Ligands which Are Hosts for Inclusion Complexes-. Crown ethers and coronands, cryptates and cryptands, calixarenes, hemispherands, and spherands, carcerands, hemicarcerands and novel `molecular flasks' enabling preparation and stabilization of short-lived species, cyclodextrins, and their Complexes, endohedral fullerene complexes, nanotubes and other fullerene-based supramolecular systems, dendrimers, cyclophanes and steroids forming inclusion complexes, anion binding receptors and receptors with multiple binding Sites.

### **UNIT-V**

(iii) Physical methods in supramolecular chemistry: Spectroscopy in supramolecular chemistry, determinationofstoichiometry, stabilityconstants, and geometry of complexes, binding constant determination, dynamics of supramolecular systems(solidstate vs solutionbehavior). (iv) Application of supramolecular chemistry: Supramolecules in catalysis as membrane transport, sensors, phase-transfer catalysts, supramolecular devices and swiches, memories, logic gates and related systems, molecular scale machines (mechanical rotors, gears andbrakes), conversion of light into fuels and light into electricity.

#### Suggested texts and References:

1. H.R. Allcock, F.W. Lampe and James Mark, Contemporary Polymer Chemistry, Prentice Hall, Inc. (1990).

2. M.P. Stevens, Polymer Chemistry: An Introduction (2nd Edition) Oxford University Press 91990).

3. F.W. Billmeyer, Jr., Textbook of Polymer Science (3rd Edition) Wiley-Inter Science (1984) paperback.

4. A. Ravve, Principles of Polymer Chemistry.

MCM r.Shaik Basha r.ch institute) External member (Academics)

5. Recommended Review Articles in the field of supramolecular chemistry.

Dr. Sumon Chand

- 6. "Supramolecular Chemistry" by F. Vogtle, John Wiley, 1991.
- 7. "Crystal Engineering. The Design of Organic Solids" by G.R. Desiraju, Elsevier, 1989.

8. Introduction to Supramolecular Chemistry, Dodzuick Helena.

### C 803: Reaction dynamics

(45 + 15 = 60 hrs.)

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#### **UNIT-I**

Chain reactions: general treatment, activation energy, chain length, chain transfer reactions, inhibition, bond dissociation energies, branching chain reactions.

### **UNIT-II**

The collision theory: Dynamics of bimolecular collisions and rate and rate constant of bimolecular reaction, factors determining effectiveness of collisions, Termolecular reactions, unimolecular reactions. Relation between cross section and rate coefficients.

### **UNIT-III**

Kinetics of fast reactions, flow methods for fast reaction, pulse methods, flash photolysis, pulse radiolysis, molecular reaction dynamics, potential energy surfaces, theoretical calculation of the rate constant, Kinetics and mechanism of photochemical reactions.

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## UNIT-IV

**Potential Energy Surfaces:** Long range, empirical intermolecular and molecular binding potentials, Internal coordinates and normal modes of vibration, Potential energy surfaces, ab- initio calculation of potential energy surface, experimental determination of potential energy surfaces.

#### UNIT-V

**Transition State Theory (TST):** Basic postulates and derivation of TST, dynamical derivation of TST, Thermodynamic formulation of TST, Application of TST

#### Suggested texts and References:

(1) J.I. Steinfeld, J.S. Francisco and W.L. Hase, Chemical Kinetics and Dynamics, Prentice Hall 1989.

(2) Paul L. Houston, Chemical Kinetics and reaction dynamics.

(3) R.D.Levine and R.B.Bernstein, Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, 1987.

(4) Sanjay K. Upadhay, Chemical kinetics and Reaction Dynamics, Springer, 2006

## C-804 Heterocyclic Chemistry

#### (45 + 15 = 60 hrs.)

**Introduction to Heterocycles**: Nomenclature (Hantzsch Widman System), spectral characteristics, reactivity and aromaticity of monocyclic, fused and bridged heterocycles.

**Nonaromatic heterocycles:** Different types of strains, interactions and conformational aspects on nonaromatic heterocycles. Synthesis, reactivity, and importance of the following ring systems. Azirines, Oxaranes, Thiiranes, Diazirenes, Diaziridines, Azetidines.

**Five and six-membered heterocycles with two hetero atoms**: Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Pyrimidine, Pyrazine, Oxazine, and Thiazine.

**Heterocycles with more than two hetero atoms:** Synthesis, reactivity, aromatic character and importance of the following heterocycles: Triazoles, Oxadiazoles, Thiadiazoles, Triazines.

**Larger ring and other heterocycles:** Synthesis and reactivity of Azepines, Oxepines and Thiepines. Synthesis and rearrangement of Diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines, and Azonines.

**Banzanellated azoles and dipolar structures**: Banzanellated azoles: Synthesis and reactivity of Benzimidazoles, Benzoxazoles and Benzothiazoles. Heterocyles with Ring-Junction nitrogen: Synthesis and reactivity of Quinolizines, Indolizines and Imidazopyridines. Heterocycles with Dipolar structures: Betaines: Formation, aromaticity and reactivity of pyridine-N-oxides and pyridinium imides. Mesoionic heterocycles: Synthesis and aromaticity of sydnones and 1,3-dipolar addition reaction of mesoionic heterocycles.

## **Recommended books:**



- 1. Heterocyclic Chemistry, T. L. Gilchrist.
- 2. An Introduction to the Chemistry of Heterocyclic compounds, R. M. Acheson.
- 3. Heterocylic chemistry, J. A. Joule & K. Mills.
- 4. Principals of Modern Heterocyclic Chemistry, A. Paquette.
- 5. Heterocyclic Chemistry, J. A. Joule & Smith.
- 6. Handbook of Heterocyclic Chemistry, A. R. Katritzky

## FIFTH YEAR SEMESTER –IX

Subject Code	Subject	Contact Hours / Week	Credits
CPr901	Project	-	20

20 (220 of 240 Credits)

## **SEMESTER –X**



Subject Code*	Subject	Contact Hours / Week Theory+Tutorials	Credits
CE1	Environmental Chemistry	[4 + 1]	5
CE2	Inorganic Rings, Cages and Clusters	[4+1]	5
CE3	Medicinal Chemistry	[4+1]	5
CE4	Nanoscience and Technology	[4+1]	5
CE5	Surface and Colloidal Chemistry	[4+1]	5
CE6	Computational Chemistry	[4+1]	5
CE7	Advanced Polymer Chemistry	[4+1]	5
	(240 of 240 credits)	Total	20
		20	

(240 of 240 credits)

# \*Four Subjects will be offered according to the availability of instructors and minimum number of interested students taking a course. The chosen four subjects will have codes CE1001, CE1002, CE1003 and CE1004.

## **CE1-** Environmental Chemistry

**Scope:** Environmental pollution, structure of atmosphere, biogeological cycles – oxygen, nitrogen, carbon, phosphorous, sulphur ; biodistribution of elements, air pollutions - reactions in atmosphere, primary pollutants, air quality standards, analysis of CO, nitrogen oxides, sulphur oxides, hydrocarbons and particulate matter, particulate pollution - control methods, vechicular pollution, green house effect and global warming, climatic changes, ozone, photochemical smog, acid rain, sampling, monitoring & control.

**Hydrosphere:** Water pollution, hydrological cycle, chemical composition, sea water composition, water quality criteria for domestic and industrial uses, BIS and WHO standards, ground water pollution, surface water pollution - lake and river water, eutrophication, marine pollution, water pollutants - biodgradeability of detergents – pestisides - endosulfan and related case studies.

**Classification of industrial waste waters:** Principles of water and waste water treatment - aerobic and anaerobic treatment, industrial waste water treatment, heavy metal pollution, hard water - softening - purification of water for drinking purposes, water treatment for industrial use, electrodialysis, reverse osmosis, other purification methods, chemical speciation of elements.



**Water analysis**: Color, odor, conductivity, TDS, pH, acidity, alkalinity, chloride, residual chlorine, hardness, trace metal analysis, elemental analysis, ammonia, nitrite, nitrate, fluoride, sulphide, phosphate, phenols, surfactants, BOD, COD, DO, TOC, nondispersive IR spectroscopy, anode stripping, ICP, AES, Chromatography, ion selective electrodes, neutron activation analysis.

**Soil pollution:** Soil humus, soil fertility, inorganic and organic components in soil, acid, base and ion exchange reactions in soils, micro and macro nutrients, wastes and pollutants in soil, introduction to geochemistry, solid waste management, treatment and recycling soil analysis, radioactive pollution, disposal of radioactive waste.

## **References:**

1. H. Kaur, Environmental Chemistry, 6th Edn, Pragathi Prakashan, Meerut, 2011.

2. K.H.Mancy and W,.J.Weber Jr. Wiley, Analysis of Industrial Waste Water, Interescience New York, 1971.

3. L.W. Moore and E. A. Moore, Environmental Chemistry, McGraw Hill Publication, New York, 2002.

4. S. M. Khopkar, Environmental Pollution Analysis, New Age International (P) Ltd, 1993.

5. Colid Baird. Environmental Chemistry, W. H. Freemand and Company, 1995.



## **CE2-** Inorganic Rings, Cages and Clusters

**Main group clusters:** Geometric and electronic structure, three - four and higher connectclusters, the closo-, nido-, arachno- borane structural paradigm, Wade-Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity.

**Transition metal clusters:** Low nuclearity metal carbonyl clusters and 14n+2 rule, high nuclearity metal carbonyl clusters with internal atoms, structure, synthesis and reactivity - capping rules.

**Isobal analogy**: Heteronuclear clusters - carboranes and heteroboranes, metal clusters - structural prediction of organometallic clusters, main group transition metal clusters: Isolobal analogs of p-block and d-block clusters - interstitial systems - cubanes and zintl clusters.

**Inorganic homo- & heterocycles:** Synthesis, structure and reactivity - structural variety & properties of borazins and phosphazenes, borides, carbides, silicides, nitrides, phosphides, oxides and sulphides of transition elements, multiple bonds and cluster variety of transition metals.

**Inorganic rings and polymers**: Definition, variety and merits, P, Si, S, N, & O based polymers, poly-phosphazenes, poly-thiazenes, poly-siloxanes and poly-silanes.

#### **References:**

1. D. M. P. Mingos and D. J. Wales, Introduction to Cluster Chemistry, Prentice Hall, 1990.

2. N. N. Greenwood and E. A. Earnshaw, Chemistry of Elements, Pergaman Press, 1984.

3. I. Haiduc & D. B. Sowerby (Eds.), Inorganic Homo-and Heterocycles Vols. 1 & 2, Academic Press, 1987.
4. J. E. Mark, R. West & H. R. Allcock, Inorganic Polymers, Academic Press, 1992.
5. T. P. Fehlner, J. F. Halet and J-Y. Saillard, Molecular Clusters: A Bridge to Solid-State Chemistry, Cambridge University Press, 2007.

6. P. Braunstein, L. A. Oro, P. R. Raithby, Ed. Metal Clusters in Chemistry, John Wiley and sons, 1999.

7. T. Chivers, I. Manners, Inorganic Rings and Polymers of the p-Block Elements, from Fundamentals to Applications, RSC Publishing, 2009.



## **CE3-** Medicinal Chemistry

**Introduction:** History of medicinal chemistry, general mechanism of drug action on lipids, carbohydrates, proteins and nucleic acids, drug metabolism and inactivation, receptor structure and sites, drug discovery development, design and delivery systems, gene therapy and drug resistance.

**Classification:** Drugs based on structure or pharmacological basis with examples, synthesis of important drugs such as  $\alpha$  - methyl dopa, chloramphenicol griseofulvin, cephelosphorins and nystatin. Molecular modeling, conformational analysis, qualitative and quantitative structure activity relationships.

**General introduction to antibiotics:** Mechanism of action of lactam antibiotics and non lactam anti biotics, antiviral agents, chemistry, stereochemistry, biosynthesis and degradation of penicillins - An account of semisynthetic penicillins, acid resistant, penicillinase resistant and broad spectrum semisynthetic penicillins.

**Elucidation of enzyme structure:** Mechanism, kinetic, spectroscopic, isotopic and stereochemical studies. Chemical models and mimics for enzymes, design, synthesis and evaluation of enzyme inhibitors.

**Interactions:** DNA-protein interaction and DNA-drug interaction. Introduction to rational approach to drug design, physical and chemical factors associated with biological activities, mechanism of drug action.

## **Recommended books:**

1. I. Wilson, Giswald and F. Doerge, Text Book of Organic Medicinal and Pharmaceutical Chemistry, J.B. Lippincott Company, Philadelphia, 1971.

2. A. Burger, Medicinal Chemistry, Wiley Interscience, New York, Vol. I and II, 1970.

3. Bentley and Driver's Text Book of Pharmaceutical Chemistry revised by L.M. Artherden, Oxford University Press, London, 1977.

4. A. Gringauz, Introduction to Medicinal Chemistry, How Drugs Act and Why?, John Wiley and Sons, 1997.

5. G. L. Patrick, Introduction to Medicinal Chemistry, Oxford University Press, 2001.



## **CE4-** Nanoscience and Technology

**Introduction to nanoscience and nanotechnology:** Underlying physical principles of nanotechnology, Nanostructured Materials, Size is Everything: Fundamental physicochemical principles, size dependence of the properties of nanostructured matter, quantum confinement, single electron charging, the central importance of nanoscale morphology, Societal aspects of nanotechnology: Health, environment, hype and reality.

**The advent of the nanomaterial:** Top down and bottom up approaches to building materials, Properties of nanomaterials such as nanoparticles, carbon nanotubes, Overview of selfassembly, Inert gas condensation, arc discharge, RF plasma, plasma arc technique, ion sputtering, laser ablation, laser pyrolysis, ball milling, molecular beam epitaxy, chemical vapour depositionmethod and electro deposition.

**The basic tools of nanotechnology:** Scanning electron microscopy (SEM), TEM and EDAX analysis and X-ray diffraction, A brief historical overview of atomic force microscopy (AFM) and an introduction to its basic principles & applications, Optical microscope and their description, operational principle and application for analysis of nanomaterials, UV-VIS-IR spectrophotometers, Principle of operation and application for band gap measurement.

**Metal nanoparticles:** Size control of metal nanoparticles and their characterization, study of their properties, optical, electronic, magnetic. Surface plasmon band and its applications, role in catalysis, alloy nanoparticles, stabilization in sol, glass, and other media, change of band gap, blue shift, colour change in sol, glass, and composites, plasmon resonance.

**Carbon nano structures:** Introduction, Fullerenes, C60, C80 and C240 nanostructures, Properties & applications (mechanical, optical and electrical), Functionalization of carbon nanotubes, reactivity of carbon nanotubes, Nanosensors: Temperature sensors, smoke sensors, sensors for aerospace and defense. Accelerometer, pressure sensor, night vision system, nano tweezers, nano-cutting tools, integration of sensor with actuators and electronic circuitry biosensors.

## **Recommended books:**

1. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill, New Delhi, 2007.

2. G. Cao, Nanostructures and Nanomaterials – Synthesis, Properties and Applications, Imperial College Press, London, 2004, chapters 3, 4 and 5.

3. C. N. R.Rao, A. Muller and A. K. Cheetham, The Chemistry of Nanomaterials, Volume 1, Wiley –VCH Verlag GmbH & Co. KgaA, Weinheim, 2004, Chapter 4



## **CE5-** Surface and Colloidal Chemistry

**Surface and Interface Chemistry:** Classifications, micellization, CMC and its determination. Shape and structure of micelles, effect of additives on micellization, thermodynamics of micellization, solubilization and applications, effect of electrolytes on solubilization. Macro and micro emlusions, dispersion and aggregation of solids by surfactants.

**Membranes and their applications:** Artificial and natural membranes, Donnan membrane equilibrium, transport of electrolytes, membrane potential and ion selective electrodes.

Adsorption on solids and porous materials: Model for multilayer adsorption, BET isotherm and application to different types of adsorbents, adsorption by porous, non-porous and microporous solids, Estimation of specific surface area and pore size distribution.

**Colloid systems and their properties:** Origin of the charges, electro-kinetic phenomena, electrophoresis, electroosmosis, sedimentation and streaming potential. The concept of electrical double layer and various models to explain its structure and properties, DLVO theory and stability of colloids. Smoluchowski theory of kinetics of coagulation and distribution of colloids aggregates. Organic and inorganic gels and clay colloids.

**Methods to detect interfacial phenomena:** Principle and instrumentation of ATR-FTIR spectroscopy, SFG Spectroscopy.

## **Recommended books:**

1. Hunter, R.J., "Foundation of colloid Science", Oxford University, Press, 2009

2. Lyklema, J., *"Fundamentals of Interface and Colloid Science"*, Academic press San Diego, 2000

3. Adamson, A.W., "Physical Chemistry of Surface",5<sup>th</sup> Ed.,Jhon Wiley and Sons, NewYork, 1990

3. Kruyt, H.R., "Colloid Chemistry" Vol. I and II. Elsevier Press, 1991

4. Gerg, S.J. and Singh, K.S.W., "Adsorption, Surface Area and Porosity", 2<sup>nd</sup> Ed., Academic Press., U.K. 1982.



## **CE6-** Computational Chemistry

**Fundamentals of electronic structure:** Basis function-hydrogen-like, Slatertype and Gaussian type orbitals, classification of basis sets – minimum, double zeta, triple zeta, split-valence, polarization and diffuse basis sets, correlation consistent basis sets, basis set super position error, energy minimization methods-derivative and non-derivative methods-simplex method, steepest descents method, Newton-Rapshon method, minima, maxima and saddle points.

**Semi empirical and Abinitio methods:** Approximation methods, self-consistent field treatment of polyatomic molecules, closed shell systems-restricted Hartree-Fock calculations, open shell systems ROHF and UHF calculations, The Roothan –Hall equations, Koopman's theorem, HF limit and electron correlation, introduction to post Hartree- Fock and density functional methods.

**Electronic properties:** Dipole moments, electrostatic potential, frequencies, population analysis, Mulliken and Lowdin analysis, solvent effects, polarizable and nonpolarizabel models.

**Introduction to simulation methods:** Molecular mechanics, Monte carlo and molecular dynamics simulations, periodic boundary conditions, radial distribution function, calculation of thermodynamics properties.

#### Suggested texts and References:

(1) C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, John Wiley & Sons, 2002.

(2) David Young, Computational Chemistry: A practical Guide for applying Techniques to Real World Problems, Wiley Interscience, 2001.

(3) A.R. Leach, Molecular Modelling: Principles and Applications, Pearson Education, 2001.

(4) J. B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods. Gaussian Inc., 1996.

- (5) M.P. Allen and D.J. Tildesley, Computer Simulations of Liquids, Oxford, 1987.
- (6) F. Jensen, Introduction to Computational Chemistry, John Willey & Sons Ltd, 1999.
- (7) A. Leach, Molecular Modeling : Principles and Applications, Prentice Hall, 2001.

(8) I. N. Levine, Quantum Chemistry, 7<sup>th</sup> Ed., PHI Learning Pvt. Ltd., Delhi, 2013.



## **CE7- Advanced Polymer Chemistry**

**Properties of commercial polymers** Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers – Fire retarding polymers and electrically conducting polymers, Bio-medical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells

**Polymer Additives:** Role of additives in polymers, Fillers, plasticizers, anti-oxidants and stabilizers, Flame-retardants, colourants.

**Natural polymers: Cellulose:** Cellulose nitrate, cellulose acetate. viscose rayon, starch, silk, Rubber and modified rubber.

**Polymer supported reagents in organic chemistry**: Preparation and application of polymer supported catalysts, acids, bases, phase transfer catalysts, transition metal complexes etc. Polymer supported reagents and polymer supported protecting groups including "Solid Phase" peptide synthesis.

**Polymer Degradation and Stabilization:** Types of degradation – Physical and chemical degradation.

**Types of Physical degradation:** a)Thermal degradation b) Photodegradation and stabilization c) Mechanical degradation.

**Types of Chemical degradation:** a) Solvolytic degradation b) hydrolytical degradation c) Oxidative degradation and stabilization d) biodegradation.

## **Recommended books:**

- 1. Text book of Polymer science ; F.w.Billmeyer J.Willey
- 2. Polymer science, V.R.Gowarikar, N.V.Vishwanathan and J.Sreedhar, Wiley Eastern
- 3. Principles of Polymerization, George Odian III.Ed.
- 4. Organic Polymer Chemistry, K.J.Saunders
- 5. Polymer Chemistry, Golding
- 6. Principles of Polymer Chemistry, Flory
- 7. Physical Chemistry of Macromolecules, D.D.Deshpande, Vishal Publications, 1985
- 8. Functional monomers and polymers, K.Takemoto, V.Inaki and R.M.Ottanbrite
- 9. Contemporary polymer chemistry, H.R.alkock and F.W.Lambe, Prentice Hall
- 10. Physics and Chemistry of polymers, J.M.G.Cowie, Blackie Academic and Professional.



## Scheme of Examination (Chemistry Stream)

Subject Code	Subject	Intern	al Marks	Externa	l Marks	Total Marks	Credit
		Max	Min	Max	Min	Max	
B101	Biology - I	60	24	40	16	100	3
C101	Chemistry - I	60	24	40	16	100	3
M101/MB101	Mathematics - I	60	24	40	16	100	3
P101	Introductory Physics- I	60	24	40	16	100	3
G101	Computer Basics	60	24	40	16	100	3
H101	Communication Skills	60	24	40	16	100	2
Practical							•
BL101	Biology Laboratory-I	60	24	40	16	100	2
CL101	Chemistry Laboratory-I	60	24	40	16	100	2
PL101	Physics Laboratory-I	60	24	40	16	100	2
GL101	Computer Laboratory	60	24	40	16	100	2
Additional P	apers	•		•	•	•	•
ES101	Environmental Studies	60	24	40	16	100	2

## Integrated M.Sc. Semester – I

## Integrated M.Sc. Semester – II

Subject Code	Subject	Intern	al Marks	Externa	l Marks	Total Marks	Credit
		Max	Min	Max	Min	Max	
B201	Biology - II	60	24	40	16	100	3
C201	Chemistry - II	60	24	40	16	100	3
M201/MB201	Mathematics-II	60	24	40	16	100	3
P201	Introductory Physics-II	60	24	40	16	100	3
G201	Electronics and Instrumentation	60	24	40	16	100	3
Practical						·	
BL201	Biology Laboratory- II	60	24	40	16	100	2
CL201	Chemistry Laboratory- II	60	24	40	16	100	2
PL201	Physics Laboratory- II	60	24	40	16	100	2
GL201	Electronics Laboratory	60	24	40	16	100	2
H201	Communication Skills Lab -I	60	24	40	16	100	2
Additional P	apers						
ES201	Environmental Studies	60	24	40	16	100	2















Subject Code	Subject	Interna	al Marks	Externa	l Marks	Total Marks	Credit
		Max	Min	Max	Min	Max	
CB301	Essential mathematics for Chemistry and Biology	60	24	40	16	100	4
CB302	Biochemistry-I	60	24	40	16	100	4
CB303	Organic Chemistry-I	60	24	40	16	100	4
C301	Inorganic Chemistry-I	60	24	40	16	100	4
H301	Creative Hindi	60	24	40	16	100	2
H302	History and Philosophy of Science	60	24	40	16	100	2
Practical							
CL301	Chemistry Laboratory	60	24	40	16	100	3
GL301	Applied Electronics Laboratory	60	24	40	16	100	2

## Integrated M.Sc. Semester – III

## Integrated M.Sc. Semester – IV

Subject Code	Subject	Intern	al Marks	Externa	l Marks	Total Marks	Credit
		Max	Min	Max	Min	Max	
PCB401	Chemical Kinetics	60	24	40	16	100	4
CB401	Introductory Spectroscopy (UV-vis, fluorescence, IR, Raman, NMR)	60	24	40	16	100	4
C401	Properties of Matter	60	24	40	16	100	3
C402	Group theory	60	24	40	16	100	3
G401	Statistical Techniques and Applications	60	24	40	16	100	4
Practical							
CL401	Chemistry Laboratory	60	24	40	16	100	3
GL401	Computational Laboratory and Numerical Methods	60	24	40	16	100	2
H401	Communication Skills Lab-II	60	24	40	16	100	2











Subject Code	Subject	Interna	al Marks	External Marks		Total Marks	Credit
		Max	Min	Max	Min	Max	
CB501	Analytical Chemistry	60	24	40	16	100	4
C501	Quantum Chemistry	60	24	40	16	100	5
C502	Inorganic Chemistry II	60	24	40	16	100	4
C503	Organic Chemistry II	60	24	40	16	100	5
H501	Scientific Writing in Hindi	60	24	40	16	100	2
Practical		<u> </u>			·	•	
CL501	Chemistry Laboratory	60	24	40	16	100	5

## Integrated M.Sc. Semester – V

## Integrated M.Sc. Semester – VI

Subject Code	Subject	Interna	al Marks	External Marks		Total Marks	Credit
		Max	Min	Max	Min	Max	
CB601	Biophysical Chemistry	60	24	40	16	100	4
C601	Atomic and molecular spectroscopy	60	24	40	16	100	3
C602	Inorganic Chemistry III	60	24	40	16	100	3
C603	Organic Chemistry III	60	24	40	16	100	4
C604	Nuclear Chemistry	60	24	40	16	100	4
H601	Ethics of Science and IPR	60	24	40	16	100	2
H602	Scientific Writing in English	60	24	40	16	100	2
Practical							
CL601	Chemistry Laboratory	60	24	40	16	100	3













Subject Code	Subject	Intern	al Marks	Externa	l Marks	Total Marks	Credit
		Max	Min	Max	Min	Max	
C701	Photochemistry	60	24	40	16	100	4
C702	Chemical biology	60	24	40	16	100	4
C703	Organometallics & Bio- inorganic Chemistry	60	24	40	16	100	4
C704	Physical Organic Chemistry	60	24	40	16	100	4
CPr701	Reading Project	60	24	40	16	100	4
Practical							
CL701	Advanced Chemistry Laboratory - I	60	24	40	16	100	5

## Integrated M.Sc. Semester – VII

Integrated M.Sc. Semester – VIII

Subject Code	Subject	Interna	al Marks	External Marks		Total Marks	Credit
		Max	Min	Max	Min	Max	
C801	Chemistry of Materials	60	24	40	16	100	4
C802	Macro and Supra-molecular chemistry	60	24	40	16	100	4
C803	Reaction Dynamics	60	24	40	16	100	4
C804	Heterocyclic Chemistry	60	24	40	16	100	4
Practical	1						•
CL801	Advanced Chemistry Laboratory- II	60	24	40	16	100	5
CPr801	Project	60	24	40	16	100	4













## Integrated M.Sc. Semester – IX

Subject	Pro Report/Di		Seminar Pro		Project R	e Based on Report and Ninar	Total Marks	Credit
CPr901-	Max	Min	Max	Min	Max	Min	Max	
Project	150	60	150	60	100	40	400	20

## Integrated M.Sc. Semester – X

Subject Code	Subject	Internal Marks		External Marks		Total Marks	Credit
		Max	Min	Max	Min	Max	
	Elective subjects will be	60	24	40	16	100	5
	offered according to the availability of instructors	60	24	40	16	100	5
CE1003	and minimum number	60	24	40	16	100	5
	of interested students taking a course from the list of elective subjects in the syllabus.	60	24	40	16	100	5



## PT. RAVISHANKAR SHUKLA UNIVERSITY

## **Centre for Basic Sciences**

## **Outcome Based Curriculum**

## **Integrated M. Sc.: Chemistry Stream**

[Choice and Credit Based System]

(Semester-I to X)

## **SESSION 2022-2023**



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## Vision & Mission

- Establish scientific institutions of the highest caliber where teaching and education are totally integrated with state-of the- art research. Make learning of basic sciences exciting through excellent integrative teaching driven by curiosity and creativity.
- Entry into research at an early age through a flexible borderless curriculum and research projects and to develop the researcher and scientist in chemical sciences through Integrated M.Sc. program.
- To develop the competent manpower with technology based experimentation, methodologies and value based practices for business and industries.

## **Objectives**

The CBS model of education is concept-based and inquiry-driven, as opposed to the more traditional content-based models. There is a strong emphasis on the interdisciplinary nature of today's science, and recognition of the importance of research experience in undergraduate education.

Courses offered in the Int. M. Sc. program at CBS form part of a comprehensive program that will enable the students-

- To understand the basic laws of nature and develop necessary skills to apply them to any desired area or discipline.
- To undertake projects to solve field base problems.
- To provide student centric learning facilities for the development of overall personality of learner. The program is planned as student-centric collaborative learning.
- Students get trained for a career in basic sciences or any related applied science or technology.



## **<u>Title of the Program: Integrated Master of Science in Chemistry</u>**

## :Program Educational Objectives:

**PEO1:** To have advance knowledge of chemistry domain.

**PEO2:** To opt for higher education, disciplinary & multi-disciplinary research and to be a lifelong learner.

**PEO3:** To provide the professional consultancy and research support and professional services from industry, research organization and recognized institutes to provide the super specialization of their domain.

PEO4: To provide, value based and ethical leadership in professional as well as social life.

## :Program Learning Outcomes:

- Students will have a firm foundation in the fundamentals and application of current chemical and scientific theories including those in Analytical, Inorganic, Organic and Physical Chemistries.
- Students will be able to design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.
- Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- Students will be able to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.
- Students will be able to explore new areas of research in both chemistry and allied fields of science and technology.
- Students will appreciate the central role of chemistry in our society and use this as a basis for ethical behavior in issues facing chemists including an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health and medicine.
- Students will be able to explain why chemistry is an integral activity for addressing social, economic, and environmental problems.

Students will be able to function as a member of an interdisciplinary problem solving team.



## :General Pattern of the Program:

Courses offered during the first year (Semesters I to II) are meant as basic and introductory courses in Biology, Chemistry, Mathematics, Physics and Environmental Science. These are common and mandatory for all students. These courses are intended to give a flavor of the various approaches and analyses and to prepare the students for advanced courses in later years of study. In addition, there will be Interdisciplinary Courses for computational skills and mathematical methods. Students are also given training to develop skills in Communication, Creative & Technical Writing and History of Science through courses in Humanities and Social Sciences.

In the second year (Semester - III), students have the freedom to choose their stream for masters program on the bases of their interest. Courses offered in the first two years would help them make an informed judgment to determine their real interest and aptitude for a given subject.

One of the important features that the CBS has adopted is semester-long projects called Lab Training / Theory projects, which are given the same weightage as a regular course. By availing this, a student can work in an experimental lab or take up a theory project every semester. This is meant to help the student get trained in research methodology, which will forma good basis for the 9<sup>th</sup> semester project work in the fifth year. The subjects/courses are describedfurther with their credit points. Few courses are common to different streams.



## FIRST YEAR SEMESTER –I

Subject Code	Subject	Contact Hours / Week Theory +Tutorials	Credits
B101	Biology – I	[2+1]	3
C101	Chemistry – I	[2+1]	3
M101/MB101	Mathematics – I	[2+1]	3
P101	Physics – I	[2+1]	3
G101	Computer Basics	[2+1]	3
H101	Communication Skills	[2]	2
	Contact Hours /Week	Laboratory	
PL101	Physics Laboratory – I	[4]	2
CL101	Chemistry Laboratory – I	[4]	2
BL101	Biology Laboratory – I	[4]	2
GL101	Computer Laboratory	[4]	2
		(25 of 240 credits)	Total: 25
Additional Paper	rs		
ES101	Environmental Studies	[2]	2

## **Semester- II**

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
B201	Biology – II	[2+1]	3
C201	Chemistry – II	[2+1]	3
M201/ MB201	Mathematics – II	[2+1]	3
P201	Physics – II	[2+1]	3
G201	Electronics and Instrumentation	[2+1]	3
	Contact Hours /Week L	aboratory	
PL201	Physics Laboratory – II	[4]	2
CL201	Chemistry Laboratory – II	[4]	2
BL201	Physics Laboratory – II	[4]	2
GL201	Electronics Laboratory	[4]	2
H201	Communication Skills Lab	[4]	2
	(50of 240 credits)	Total	25
Additional Paper			
ES201	<b>Environmental Studies</b>	[2]	2



## SECOND YEAR Semester- III

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
CB301	Essential mathematics for Chemistry and Biology	[3+1]	4
CB302	Biochemistry-I	[3+1]	4
CB303	Organic Chemistry-I	[3+1]	4
C301	Inorganic Chemistry-I	[3+1]	4
H301	Creative Hindi	[2+0]	2
H302	History and Philosophy of Science	[2+0]	2
	Contact Hours / Week Laboratory	·	
CL301	Chemistry Laboratory	[6]	3
GL301	Applied Electronics Laboratory	[4]	2
	(75 of 240 credits)	Total	25

## **Semester- IV**

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
PCB401	Chemical kinetics	[3+1]	4
CB401	Introductory Spectroscopy (UV-vis, fluorescence, IR, Raman, NMR)	[3+1]	4
C401	Properties of Matter	[2+1]	3
C402	Group theory	[2+1]	3
G401	Statistical Techniques and Applications	[3+1]	4
		Lab hrs	Credits
CL401	Chemistry Laboratory	[6]	3
GL401	Computational Laboratory and Numerical Methods	[4]	2
H401	Communication Skills Lab	[4]	2
	(100 of 240 credits)	Total	25



## THIRD YEAR

## Semester- V

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
CB501	Analytical Chemistry	[3+1]	4
C501	Quantum Chemistry	[3+2]	5
C502	Inorganic Chemistry II	[3+1]	4
C503	Organic Chemistry II	[3+2]	5
H501	Scientific Writing in Hindi	[2]	2
		Lab contact hrs	Credits
CL501	Chemistry Laboratory	[10]	5
	(125 of 240 credits)	Total	25

## Semester- VI

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
CB601	Biophysical Chemistry	[3+1]	4
C601	Atomic and molecular spectroscopy	[2+1]	3
C602	Inorganic Chemistry III	[2+1]	3
C603	Organic Chemistry III	[3+1]	4
C604	Nuclear Chemistry	[3+1]	4
H601	Ethics in Science and IPR	[2+0]	2
H602	Scientific Writing in English	[2]	2
		Lab contact hrs	Credits
CL601	Chemistry Laboratory	[6]	3
	(150 of 240 credits)	Total	25



## FOURTH YEAR

## Semester- VII

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
C701	Photochemistry	[3+1]	4
C702	Chemical biology	[3+1]	4
C703	Organometallics & Bio-inorganic Chemistry	[3+1]	4
C704	Physical Organic Chemistry	[3+1]	4
CPr701	Reading project	-	4
		Lab contact hrs	Credits
CL701	Advanced Chemistry Laboratory-I	[10]	5
	(175 of 240 credits)	Total	25

## **Semester- VIII**

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
C801	Chemistry of Materials	[3+1]	4
C802	Macro and Supra-molecular chemistry	[3+1]	4
C803	Reaction Dynamics	[3+1]	4
C804	Heterocyclic Chemistry	[3+1]	4
		Lab contact hrs	Credits
CL801	Advanced Chemistry Laboratory-II	[10]	5
CPr801	Project	-	4
	(200 of 240 credits)	Total	25



## **FIFTH YEAR**

## Semester- IX

Subject Code	Subject	Contact Hours / Week	Credits
CPr901	Project		20
	(220 of 240 Credits)	Total	20

## Semester- X

Subject Code*	Subject	Contact Hours / Week Theory+Tutorials	Credits
CE1	Environmental Chemistry	[4+1]	5
CE2	Inorganic Rings, Cages and Clusters	[4 + 1]	5
CE3	Medicinal Chemistry	[4 + 1]	5
CE4	Nanoscience and Technology	[4+1]	5
CE5	Surface and Colloidal Chemistry	[4+1]	5
CE6	Computational Chemistry	[4 + 1]	5
CE7	Advanced Polymer Chemistry	[4 + 1]	5
	(240 of 240 credits)	Total	20

\*Four Subjects will be offered according to the availability of instructors and minimum number of interested students taking a course. The chosen four subjects will have codes CE1001, CE1002, CE1003 and CE1004.



## <u>:SEMESTER WISE COURSE OUTCOMES:</u> Int. M. Sc. Chemistry program

#### C 101: Chemistry-I

Student will gain understanding of-

- Chemistry at the level of atoms and molecules, and to make connections between the rules governing such microscopic particles to what we observe in the macroscopic world.
- Structure and properties of atoms and molecules and gives a brief introduction of physical organic chemistry.
- In addition, a part of this course also deals with bonding, hybridization.

#### CL 101: Chemistry Laboratory

- 1. To calibrate given glasswares (i) 100 ml beaker & (ii) 50 ml volumetric flask.
- 2. To calibrate given glasswares (i) Burette, (ii) Pipette & (iii) Measuring cylinder.
- 3. To calibrate given glasswares (i) Micripipette.
- 4. To determine the strength of unknown solution of NaOH with N/10 oxalic acid by volumetric.
- 5. To determine the strength of unknown solution of NaOH with N/10 hydrochloric acid by volumetric.
- 6. To determine the strength of unknown solution of NaOH with potassium hydrogen phthalate by volumetric.
- 7. To determine hardness of given water sample complexometrically using EDTA & EBT.
- 8. To determine the strength of unknown solution of magnesium salt solution using standard magnesium solution and EDTA complexometrically.
- 9. To identify functional group:
  - (i) Glucose
  - (ii) Starch
  - (iii) Carboxalic acid
  - (iv) Oxalic acid
  - (v) Benzoic acid
  - (vi) Phthalic acid



	(vii)	Acetone
	(viii)	Acetophenone
		Methanol
	(ix)	
	(x)	Ethanol
	(xi)	β- napthol
	(xii)	α- napthol
	(xiii)	Ethyl acetate
	(xiv)	Benzamide
	(xv)	Urea
	(xvi)	Thiourea
	-	arate Ni (II) & Co (II) by paper chromatography.
		stry-II
tudent	-	ain understanding of-
•		pts in chemical principles and focuses on the changes that molecules undergo through
	-	ature change.
•		o-chemistry, thermodynamics, laws, types and its application to various areas in detail
		nphasis on practical applications.
		nistry Laboratory
1.		ermine endpoint of neutralization by the conductometric titration using strong acid
		ng base.
2.	To det	ermine end point of neutralization by the conductometric titration using weak acid
	& wea	k base.
3.	To det	ermine $pK_a$ of monobasic acid using pH meter.
4.		ntify two acidic-, basic- and interfering radicals in given inorganic mixture (various nations).
5.	To det	ermine molar volume of isopropyl alcohol & its partial molar volume.
6.	To det	ermine molar volume of ethanol & its partial molar volume.
in the	External Member	Bullow Dr. Shaik Basha Research Institute) Research Institute) Res

- 7. To study the variation of viscosity with methanol & water.
- 8. To determine % composition of mixture of ethanol & water by surface tension method.
- 9. To determine % composition of mixture of methanol & water by surface tension method.
- 10. Short project of 2 weeks based on the experiments available in Journal of Chemical Education.

## CB303: Organic Chemistry-I

Student will gain understanding of-

- Structural chemistry of organic compounds with an emphasis on electronic structure, reactivity, conformation and stereochemistry.
- Various strategies involved in logical organic synthesis by incorporating basic organic transformations, reactions, and reactivity. Various functional group transformations, reagents, and reaction mechanisms, will be discussed to provide students a clear understanding and importance of organic synthesis.

This course should serve as a stepping stone for students looking to progress to more advanced synthetic concepts and methodologies. These concepts will prepare students for a mechanistic-based approach to learning organic reactivity. Emphasis will be given towards developing problem-solving skills unique to organic chemistry.

## C301: Inorganic Chemistry-I

Student will gain understanding of-

- Chemistry of main group elements such as hydrogen, alkali metals and P-block elements from group 13 18 of the periodic table. The central theme of this course is to give a detailed account on the fundamental concepts relevant to structure and bonding, acids and bases, redox behavior, reactions and applications of the main group elements and their compounds.
- In addition to providing a necessary foundation for inorganic chemistry, this course will also emphasize the role of main group compounds in multi disciplinary areas of chemistry such as supramolecular, organometallic, materials science and catalysis.

## CL301: Chemistry Laboratory

- 1. Preparation of Tetraamine Cupric Sulphate
- 2. Preparation of Potash alum



- 3. Preparation of Mohr's salt
- 4. Preparation of Epsom salt from Magnesium chloride
- 5. Preparation of Potassium trioxalate chromate (III)
- 6. Preparation of Nickel Ammonium Sulphate using Nickel Sulphate and Ammonium Sulphate
- 7. Preparation of Sodium trioxalato ferrate from ferric chloride, oxalic acid and sodium hydroxide
- 8. Preparation of Ammonium Ferric Sulphate using Ferrous Sulphate and Ammonium Sulphate
- 9. Preparation of Hexammine nickel (II) chloride
- 10. Preparation of Potassium Chlorochromate
- 11. Preparation of Cis-Potassiumdioxalatodiaquachromate
- 12. Preparation of Lead chromate
- 13. Preparation of Chrome alum
- 14. Preparation of Hexamine Cobalt (III) Chloride
- 15. Estimation of barium as barium sulphate in the given solution of barium chloride gravimetrically
- 16. Estimation of barium as barium sulphate gravimetrically and estimation of zinc volumetrical from the mixture of barium chloride and zinc oxide

## **PCB401:** Chemical kinetics

Student will gain understanding of-

- Basic concepts of chemical kinetics, theories, fundamental terms, complex reactions and derivations.
- Reactions in solutions and their kinetics too.
- Various techniques for kinetic measurements (for fast reactions) are also described (like temperature and pressure jump methods, flash photolysis).
- Catalysis and surface reactions are also discussed.

## CB401: Introductory Spectroscopy (UV-vis, fluorescence, IR, Raman, NMR)

This is a very essential module for both chemistry and biology students. Student will gain understanding of-



- Basics of spectroscopy, interaction of electromagnetic waves with matter, types of spectroscopic techniques like UV-Vis, Fluorescence spectroscopy,
- IR, Raman, Mass spectroscopy.
- Nuclear magnetic resonance spectroscopy Proton chemical shift, spinspin coupling, coupling constants and applications to organic structures 13C resonance spectroscopy is also covered etc.

## C401: Properties of Matter

Student will gain understanding of-

- Introduction of states of matter (Gas, solid, liquid etc).
- Gaseous state covers Perfect gases and gas laws, law of partial pressures and partial volumes, Graham's law of effusion, The kinetic theory of gases.
- Intermolecular forces, Vapour pressure, Surface tension, Viscosity etc are described in liquid state section.
- Solid state and colloidal state are described.

#### C402: Group theory

The objective of this course is to recognize symmetry in molecules and understand its role in chemistry. The course will explore the role of symmetry in -

- Determining molecular properties like optical activity and dipole moment
- Classifying and assigning nomenclature to molecules, molecular states and molecular motions,
- Bringing about simplifications in the application of quantum mechanics to molecules and
- Determining spectroscopic selection rules based on molecular symmetry. Group theory applied to the study of molecular symmetry has far reaching consequences in chemistry and the course will provide an in-depth appreciation of this.

## **CL401: Chemistry Laboratory**

- Study on hydrolysis of ethyl acetate catalysed by 1M of HCl at room temperature and also stu on effect of anionic surfactant SDS (sodium dodecyl sulphate)
- 2. Study on the rate of reaction of ethyl acetate at two different concentration of acid.
- 3. Study on the decomposition of  $H_2O_2$  by  $Fe^{3+}$  and  $Cu^{2+}$  at  $35^{\circ}C$ .



Other experiments related to kinetics will be performed.

## **CB501:** Analytical Chemistry

Separation plays a crucial role in Chemistry and Biology, where sample purity is of utmost importance e.g. Pharmaceuticals, Biopharmaceuticals and Fragrances etc. In this course, Student will gain understanding of-

- Theory and practice of separation.
- Various separation techniques like HPLC, GC, GC MS, Centrifugation, Electrophoresis and few other Chromatographic techniques.
- Principle, instrumentation and applications.

## C501: Quantum Chemistry

The objective of this course is to-

- Understand the rules governing the behavior of molecules and atoms the theory of quantum mechanics and thereby get a feeling for how to explain and predict chemical properties.
- The course starts by discussing the fundamental principles of quantum mechanics with an emphasis on the physical implications of this elegant, yet non-intuitive theory. It then applies quantum mechanics to simple model systems and eventually to atoms and molecules.
- It explores one of the most pervasive concepts in chemistry: the chemical bond. The ideas discussed in this course will be useful to those who wish to pursue further study in the areas of theoretical and computational chemistry, spectroscopy, molecular biology and materials science.

## C502: Inorganic Chemistry II

The objective of this course is to understand-

- Chemistry of transition metals group-wise and series-wise. The central theme of this course is to focus on the fundamental concepts.
- Transition metal chemistry relevant to their structure, bonding, properties such as spectral characteristics, reactivity, stereochemistry etc.
- Chemistry of f-block elements (lanthanide and actinide elements)

## C503: Organic Chemistry II

The module is the extension of Organic Chemistry-I and student will gain understanding of-



- Stereochemistry of organic compounds, molecular chirality and elements of symmetry.
- Mechanism and stereochemical outcome of various reactions.
- Chemistry of heterocyclic compounds and chemistry of alicyclic compounds.

## CL501: Chemistry Laboratory

**1.** Determination of concentration of  $K^+$  ion in given water sample by using flame photometer.

**2.** Conductometric study of Saponification of ethyl acetate by sodium hydroxide at equal concentration of ester and alkali at room temperature.

**3.** Determine of concentration of Na<sup>+</sup> ion in given water sample by using flame photometer.

**4.** Conductometric study of Saponification of ethyl acetate by potassium hydroxide at equal concentration of ester and alkali at room temperature.

**5.** Determination of the concentration of Fe in a sample of water using ammonium thiocyanate by spectrophotometer.

**6.** Determination of the concentration of Fe in a sample of water using 1,10\_phenanthroline by spectrophotometer.

**7.** Determination of strength of given HCl solution by titrating it potentiometrically against a solution of sodium hydroxide.

8. Isolation of lycopene from tomatoes.

**9.** Isolation of caffeine from tea leaves.

**10.** Isolation of casein and lactose from milk.

## **CB601: Biophysical Chemistry**

This course is for both chemistry and biology students and will gain understanding of-

- Different interactions those are important for the formation of structures in biological systems and
- How thermodynamic parameters can be measured and explains the basic concepts within statistical thermodynamics.
- Protein denaturation and stability, Introduction of DSC and ITC. It also includes spectroscopic methods to study of structures, functions and interactions of biomolecules.

## C601: Atomic and molecular spectroscopy

The objective of this course is to teach the fundamentals of major branches of spectroscopy and its



applications. Spectroscopy is an important research tool in all areas of science (Chemistry and Biology). Student will gain understanding of-

- Determination of structure, property and interaction of molecules. In principle, the interaction of light with matter provides a great deal of physical, chemical and biological information about a system of interest, and ultimately defines many of the observational techniques used.
- Spectroscopy topics such as EPR and Mossbauer for metal ions. In this course, this radiationmatter interaction and the quantitative information it can provide about molecular systems will be examined.

#### C602: Inorganic Chemistry III

This is the extension of Inorganic Chemistry II. Student will gain detailed understanding of-The objective of this course is to-

- Provide a detailed account to the chemistry of transition metals and emphasize their relationship to other multidisciplinary topics such as organometallic chemistry.
- The central theme of this course is to focus on the fundamental concepts needed to understand the transition metal chemistry relevant to their structure, bonding, properties such as spectral characteristics, reactivity, stereochemistry etc.

At the end of this course, students will also learn about the role of transitionmetals in several other fields like materials science, biology and catalysis.

#### C603: Organic Chemistry III

The module deals with chemistry of natural products and student will gain understanding of-

- Basics, classification and role of several natural products like alkaloids, terpenoids, steroids, natural pigments.
- Stereochemical aspects of mentioned natural products and their characteristics reactions too
- Carbohydrates: Stereochemistry, reaction and conformation and
- Chemistry of Chemistry of vitamins A, B, C and E.

#### C604: Nuclear Chemistry

Student will gain understanding of-

• Fundamental nuclear particles, nuclear structure, stable and unstable atomic nuclei, nuclear reactions.



- Different type's nuclear models and their features with nuclear reactions and their energies.
- Nuclear structure, stable and unstable atomic nuclei, different modes of radioactive decay and also methods for measurements of radioactivity.
- Fundamentals of radiochemistry, radiation chemistry and the applications.

## CL601: Chemistry Laboratory

**1.** To determine the total alkalinity in a given water sample.

**2.** To determine the CMC (Critical Micelle Concentration) of surfactant by fluorescence technique using pyrene as a probe.

**3.** Determination of Lead (Pb) in given water sample using Dithiozone by spectroscopically.

4. Determination of Molybdenum using Potassium Thiocynate by solvent extraction method.

**5.** To construct the phase diagram for three component system.

**6.** Synthesis of hexaammine cobalt(III) chloride,  $[Co(NH_3)_6Cl]^{3+}$ .

7. Synthesis of pentaammine cobalt(III) chloride.

8. Determination of the acid dissociation constant of methyl red using spectrophotometric method.

And some experiments based on analytical techniques.

## C701: Photochemistry

This course will give idea to students that-

- How light can take a major role in many natural and chemical processes. Here the students will also get through knowledge about excited state processes (e.g. fluorescence, phosphorescence etc.) and the importance of the above mentioned processes in all fields of science.
- The course also covers organic photochemistry and describes photochemistry of, pericyclic reactions and sigmatropic reactions.

## C703: Organometallics & Bio-inorganic Chemistry

This course will explore the-

- Inorganic chemistry behind the requirement of biological cells for metals such as zinc, iron, copper, manganese, and molybdenum.
- The reactivity of coordination complexes of metal ions will be discussed in the context of the reaction mechanisms of specific metalloenzymes..



## C704: Physical Organic Chemistry

The main objective of this course is to expose students to-

- Fundamental concepts of structure and function in organic reactions.
- Learn the use of kinetics and thermodynamics to elucidate mechanisms of reactions will be dealt with.
- At the end of this course, students will be in a position to predict reactivity patterns and propose reasonable mechanisms.

#### **CPr701: Reading project**

- Project is kept as a provision in CBS curriculum to give training to students and motivate to pursue research as a career.
- This is the first phase where the students are made familiar to preliminary aspect of research which starts with reading and understanding a research problem through review articles / research articles.

## CL701: Advanced Chemistry Laboratory-I

- 1. Green synthesis and characterization of silver nanoparticle (AgNPs) using leaf extract of basil (*Ocimum sanctum*).
- 2. Green synthesis and characterization of silver nanoparticle (AgNPs) using mango (*Magnifera indica*) leaf extract.
- To synthesize and characterize the CdTe quantum dots using UV-VIS and Fluorescence. Also calculate the diameter (size), Band gap and FWHM (Full Wave Half Maxima) of quantum dot.
- 4. Determination of salinity of given water sample using conductivity meter.
- 5. Determination of solubility and solubility product of sparingly soluble salt (BaSO<sub>4</sub>) conductometrically.
- 6. To determine the distribution coefficient of iodine between  $CCl_4$  and  $H_2O$  at room temperature.
- 7. To extract the essential oil of Eucalyptus citriodora leaves using Clevenger's apparatus
- 8. To extract the essential oil of ginger using Clevenger's apparatus



- 9. To extract the essential oil of *Ocimumtenuiflorum* (Tulsi) leaves using Clevenger's apparatus.
- 10. Determination of SO<sub>4</sub><sup>-2</sup> (sulphate) ion concentration in given water sample by nephloturbidity meter.
- 11. To Synthesize the Gold Nanoparticles using Tea Powder extracts.
- 12. To investigate the adsorption of acetic acid from aqueous solution by activated charcoal, verifying Freundlich and Langmuir adsorption isotherm.

#### **C801:** Chemistry of Materials

Student will gain understanding of-

- Basic aspects of the solid state, their structures, defects and types of defects.
- Thermal properties of solids and conductors. It describes High Tc Materials, Defect pervskites and their Magnetic and Optical Properties.
- Synthesis of multiphase materials, thin films and properties.
- Liquids crystals: mesmorphic behavior.

## C802: Macro and Supra-molecular chemistry

This chemistry course is aimed to provide-

- Fundamental aspects of self-assembly in chemistry and its application for supramolecular architectures.
- This course is beneficial for students who are interested in molecular materials, nanomaterials, biology-chemistry interface and self-assembly in chemical and biological systems.
- The course also consists of student's seminars on selected topics, problem solving, and idea generation and laboratory experiments on making and testing of self-assembled objects.

## **C803: Reaction Dynamics**

Reaction dynamics is a very important branch of physical chemistry; It explains-

- Why chemical reactions occur and how to predict their behavior to control them. It's closely related to chemical kinetics.
- Chain reactions, collision theory, potential energy surfaces, and details of the reaction path and molecular dynamics of few reactions as H2 + H reaction. Course also covers dynamics of transition state theory.



## C804: Heterocyclic Chemistry

Student will gain understanding of-

- Heterocyclic aromatic organic compounds, classifications and explains their reactivity based on their properties.
- Reactions and synthesis of important electron deficient nitrogen containing heterocycles; pyridines, diazines and their benzo-condenced analogs.

A mechanistic level, reactions and synthesis of important electron rich. heterocycles; furans, pyrroles and thiophenes and 1,3 azoles, and benzo-condenced analogs.

#### CL801: Advanced Chemistry Laboratory-II

#### **CPr801: Project**

- The main objective of such projects is to develop research aptitude in students at early stage.
- This is the second phase where the students will undertake some research problem and solve it through experiments.
- Further a report is submitted and presented for discussion.

#### **CPr901: Project**

- This whole semester is fully dedicated to research.
- Students will undertake six month research training from any of the recognized premier institute or university.
- The course aims to provide a full fledged exposure to students to experience fully devoted research environment, learn techniques and develop writing skills too.

## Electives for 10<sup>th</sup> Sem

#### **CE-1** (Environmental Chemistry)

This course demonstrates knowledge of-

- Chemical and biochemical principles of fundamental environmental processes in air, water, and soil and pollution.
- Basic chemical concepts to analyze chemical processes involved in different environmental problems (air, water & soil) with experimental methods for analysis of water and soil analysis and pollution.



• Classification of industrial waste waters, hard water - softening - purification of water for drinking purposes, water treatment for industrial use and Water analysis (physical and chemical parameters) in detail.

## **CE-2** (Inorganic Rings, Cages and Clusters)

This module covers advance inorganic chemistry. It describes-

- Main group clusters, transition metal clusters their synthesis and reactivity.
- Inorganic homo- & heterocycles of borides, carbides, silicides, nitrides, phosphides, oxides and sulphides of transition elements.
- Inorganic rings and polymers: Definition, variety and merits, P, Si, S, N, & O based polymers, poly-phosphazenes, poly-thiazenes, poly-siloxanes and poly-silanes etc.

## **CE-3** (Medicinal Chemistry)

This course is intended to provide insights into applications of organic chemistry in the field of drug discovery and development. Student will gain understanding of-

- History of medicinal chemistry, drug discovery and classifications.
- Approaches to lead identification followed by structure-activity determination for optimization of a drug's activity.
- Modern methods of drug delivery including formulations and prodrug approaches will be briefly discussed. Finally, we will present a brief introduction to pharmacology, target identification, pre-clinical and clinical development of a drug candidate.

## **CE-4 (Nanochemistry and Nanoscience)**

The course gives an overview of nano-science and nanochemistry. Student will gain understanding of-

- Their preparations methods, fundamental physicochemical principles, size dependence of the properties of nanostructured matter, their quantum confinement, single electron charging, the central importance of nanoscale morphology.
- Further the characterization techniques are covered with special emphasis to SEM, TEM, AFM, XRD, other spectroscopic methods etc.
- Some interesting nano-materials like metal nano-particles, quantum dots, carbon nanotubes.



## **CE-5** (Surface Chemistry)

Student will gain understanding of-

- Introduction to surface and interface chemistry with surface active reagents, their classifications and applications.
- Idea of colloidal systems and their properties and adsorption on soilds and porous materials.
- Very important research aspect of surface chemistry i.e. Membranes and their applications artificial and natural membranes, Donnan membrane equilibrium, transport of electrolytes, membrane potential and ion selective electrodes.

## **CE6-** Computational Chemistry

This module covers advance quantum chemistry and explains-

- The concept of wave function, oscillators, time dependent perturbation theory.
- Hartee-fock theory with reference to computation aspects and the electronic properties of molecules by Semi-empirical method, density functional method and configuration interaction and its limitations with applications.

## **CE7- Advanced Polymer Chemistry**

This course is very important for all the students who wish to learn and practice macromolecular and organic chemistry. Student will gain understanding of-

- Fundamental knowledge in polymer science.
- New physical chemistry concepts in macromolecules, organic synthetic methodologies for polymers and applications of polymers in the industrial applications.
- This course is beneficial for students who are interested in polymeric materials, nanomaterials, biology-chemistry interface and macromolecular assemblies in chemical and biological systems.

