

This four-semester course is an amalgamation of conventional chemistry courses such as organic, inorganic and physical chemistry with new dimensional courses such as IPR, green chemistry, polymer chemistry, medicinal chemistry and a final year research project to enhance the fundamental knowledge and research ability of the students.

CBCS Based M. Sc. Applied Chemistry Course Structure

S. No.	Code	Course Name	Category	L-T-P	Credits
Semester- I					
1.	CH 401	Physical Chemistry-I	C	4-0-0	4
2.	CH 403	Inorganic Chemistry-I	C	4-0-0	4
3.	CH 405	Organic Chemistry-I	C	4-0-0	4
4.	CH 407	Characterization Techniques-I	C	4-0-0	4
5.	CH 409	Laboratory-I	C	0-0-8	4
6.	CH 411	Laboratory-II	C	0-0-8	4
		Total		16-0-16	24
		Total Contact Hours		32	
Semester- II					
1.	CH 402	Physical Chemistry-II	C	4-0-0	4
2.	CH 404	Inorganic Chemistry-II	C	4-0-0	4
3.	CH 406	Organic Chemistry-II	C	4-0-0	4
4.	CH 408	Green Chemistry -I	C	2-0-0	2
5.	CH 410	Laboratory-III	C	0-0-8	4
6.	CH 412	Laboratory-IV	C	0-0-8	4
7.	CH 414	Computational Chemistry	AECC	0-0-4	2
8.		DSE-I(Select any one)	DSE	3-0-0	3
		Total		17-0-20	27
		Total Contact Hours		37	
Summer Training (After Semester-II)					
1.	CH 501	Summer Training (4-6 weeks duration)	C	0-0-0	2
Semester- III					
2.	CH 503	Green Chemistry-II	C	3-0-0	3
3.	CH 505	Intellectual Property Rights (IPR)	C	3-0-0	3
4.	CH 507	Laboratory-V	C	0-0-8	4
5.	CH 509	Laboratory-VI	C	0-0-8	4
6.		*Generic Elective (Select any one)	GE*	3-0-0	3
7.		DSE-II (Select any one)	DSE	3-0-0	3
8.		DSE-III(Select any one)	DSE	3-0-0	3
9.		DSE-IV (Select any one)	DSE	3-0-0	3
		Total		18-0-16	28
		Total Contact Hours		34	
Semester- IV					
1.	CH 502	Project	-	-	20
		Total credits for all semester			99
*Generic Elective (GE) (Select any one)					
1.	ES 507	Waste Management	GE	3-0-0	3
2.	ES513	Research methodology	GE	3-0-0	3

Discipline Specific Electives (DSE-I) (Select any one)					
1.	CH 416	Medicinal Chemistry -I	DSE	3-0-0	3
2.	CH 418	Biomolecules-I	DSE	3-0-0	3
3.	CH 420	Polymer-I	DSE	3-0-0	3
4.	CH 422	Bioinorganic Chemistry-I	DSE	3-0-0	3
Discipline Specific Electives (DSE-II) (Select any one)					
1.	CH 511	Medicinal Chemistry-II	DSE	3-0-0	3
2.	CH 513	Bioinorganic Chemistry-II	DSE	3-0-0	3
3.	CH 515	Polymer-II	DSE	3-0-0	3
Discipline Specific Electives (DSE-III) (Select any one)					
1.	CH 517	Catalysis	DSE	3-0-0	3
2.	CH 519	Characterization Techniques-II	DSE	3-0-0	3
3.	CH 521	Nanomaterials	DSE	3-0-0	3
Discipline Specific Electives (DSE-IV) (Select any one)					
1.	CH 523	Biomolecules-II	DSE	3-0-0	3
2.	CH 525	Some Industrial Chemicals	DSE	3-0-0	3
<i>School/Department will not be bound to run all the courses. Minimum number of students may be fixed to run any elective course.</i>					

Semester I

CH401: PHYSICAL CHEMISTRY – I

(Credits: 04, Lectures: 60)

Unit I

15L

Chemical Kinetics: Collision theory of reaction rates, the steric requirement, Arrhenius equation and activated complex theory (ACT), comparison of collision and activation complex theory, thermodynamic formulation of activated complex theory, chain reactions (hydrogen-halogen reaction), unimolecular reactions, Lindemann – Hinshelwood mechanism of unimolecular reactions.

Unit II

15L

Thermodynamics I: Recapitulation of thermodynamic laws. Maxwell relations, Gibbs-Helmholtz equation, Partial molar quantities chemical potential and Gibbs-Duhem equation, variation of chemical potential with temperature & pressure, chemical potential of ideal gases, Clapeyron-Clausius equation and its applications, Nernst heat theorem, third law of thermodynamics, entropy changes in chemical reactions.

Unit III

15L

Thermodynamics II: Ideal solutions: Raoult's law, Duhem-Margules equation and its application to vapour pressure curves (binary liquid mixture), determination of activity coefficient from vapour pressure measurement, Henry's law. Non ideal solutions: deviations from ideal behavior of liquid mixtures, liquid vapour compositions, condition for maximum.

Unit IV

15L

Electrochemistry: Debye-Hückel theory of ion-ion interaction and activity coefficient, applicability and limitations of Debye-Hückel limiting law, its modification for finite-sized ions, effect of ion-solvent interaction on activity coefficient. Physical significance of activity coefficients, mean activity coefficient of an electrolyte. Debye-Huckel-Onsager (D-H-O) theory of electrolytic conductance, Pair-wise association of ions (Bjerrum treatment), Modification of D-H-O theory to account for ion-pair formation.

Metal/Electrolyte interface, Concept of electrical double layer and its structure: Helmholtz-Perrin, Gouy-Chapman, and Stern models.

Reference books

1. S. Glasstone- Text book of Physical Chemistry 1936 .
2. G. M. Barrow –, Physical Chemistry Tata-McGraw Hill, 5th ed., 2006.
3. R. Stephen Berry, Stuart A. Rice and John Ross, Physical Chemistry 2nd ed., Oxford Univ. Press, New York, 2000
4. J.I. Steinfeld, J.S. Francisco and W.L. Hase, Chemical Kinetics and Dynamics, 2nd ed., Prentice Hall, New Jersey, 1999.
5. P. W. Atkins, and Paula, J. de Atkin's Physical Chemistry 8th ed., Oxford University Press 2006.
6. D. A. Mc Quarrie and D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt. Ltd, New Delhi, 5th ed ,2003.
7. D. A. Mc Quarrie, J. D. Simon, Molecular Thermodynamics, University Science Books, nSausalito, California, 1999.
8. HoriaMetiu, Physical Chemistry, Taylor & Francis, 2006.
9. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th ed. Wiley, 2004.
10. Physical Chemistry by Walter J Moore, Published by Prentice-Hall, 1983

CH403: INORGANIC CHEMISTRY-I

(Credits: 04, Lectures: 60)

Unit-I

15L

Coordination Chemistry-Bonding: Valence bond theory (VBT), Inner and outer orbital complexes, Crystal field theory (CFT), Crystal field stabilization energy (CFSE), Weak and strong fields complexes, Factors affecting the CFSE, Jahn Teller distortion, Applications of CFT, Molecular orbital theory (MOT) - with and without pi-bonding.

Unit-II

15L

Stability Constants and Reaction Mechanisms of Metal Complexes: Stepwise and overall formation constants and their relations, Factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand and chelate effect, Irving William series. Substitution reactions in octahedral complexes, Inert and labile complexes, VBT and CFT on inert and labile complexes, Substitution reactions in square planer complexes, Trans effect, Polarization and pi-bonding theories on trans effect.

Unit III

15L

Group Theory and its Applications - I: Symmetry elements and symmetry operation, Definitions of group and its characteristics, Subgroups, Classes and similarity transformation,

Products of the symmetry operations, Equivalent atoms and equivalent symmetry elements, Relations between symmetry elements and symmetry operation.

Unit IV

15L

Group Theory and its Applications - II: Point groups and classification, Optical activity and dipole moment, Matrix representations of groups, Reducible and irreducible representations, The great orthogonality theorem, Character tables, Direct product, Infrared and Raman spectroscopy.

Reference Books

1. J. D. Lee, Concise Inorganic Chemistry, 5thed., Elbs with Chapman and Hall, London 2008.
2. J.N. Murre, SFA Kettle and JM. Tedder, The Chemical bond, 2nd ed. Wiley, New York 1996.
3. F.A. Cotton and Wilkinson, Advanced Inorganic Chemistry, 6th ed. John Wiley 2006.
4. J.E. Huhey, Inorganic Chemistry, 4rd ed. Harper & Row, New York, 2006.
5. T. Moeller, Inorganic Chemistry, A Modern Introduction, John Wiley and Sons 1982.
6. Chemical application and Group theory, 3rd edition F.A. Cotton 2008.

CH405: ORGANIC CHEMISTRY-I

(Credits: 04, Lectures: 60)

Unit-I

15L

Reaction Mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, effect of structure on reactivity - resonance and field effects, steric effect, quantitative treatment, Linear free energy relationships (LFER), the Hammett equation - substituent and reaction constants; the Taft treatment of polar and steric effects in aliphatic compounds. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.

Unit-II

15L

Mechanism of Substitution Reactions-I

Nucleophilic Aliphatic substitution: The limiting cases SN1 and SN2, detailed mechanistic description and border line mechanisms, nucleophilicity and solvent effects, competition between nucleophilicity and basicity, ambident nucleophiles, leaving group effects, steric and other substituent effects on substitution and ionization rates, stereochemistry of nucleophilic substitution, SNi, SN1', SN2' and SNi' mechanisms.

Nucleophilic Aromatic substitution: The Aromatic SN1, SN2 and benzyne mechanisms. Reactivity – effect of substrate structure, leaving group, and attacking nucleophile.

Unit-III

10L

Mechanism of Substitution Reactions-II

Electrophilic Aliphatic Substitution: Bimolecular mechanisms - SE2 and SEi The SE1 mechanism, electrophilic substitution accompanied by double bond shifts, Effect of substrates, leaving group and the solvent polarity on the reactivity.

Electrophilic Aromatic Substitution: The Arenium ion mechanism, orientation and reactivity in mono-substituted benzene rings, ortho/para ratio. Ipso substitution.

Unit-IV

7L

Mechanism of Addition Reactions

Addition to Carbon–Carbon Multiple Bonds: Mechanism and stereochemical aspects of the addition reactions involving electrophiles and free radicals, regio and chemo-selectivity, orientation and reactivity. Hydrogenation of double and triple bonds, Hydroboration reaction, hydrogenation of aromatic rings.

Unit-V

6L

Addition to Carbon-Hetero Atoms Multiple Bonds: Hydration and Addition of Alcohols to Aldehydes, Ketones and Acids. Addition-Elimination Reactions of Ketones and Aldehydes, Reactivity of carbonyl compounds towards Addition. Hydrolysis Reactions: Ester hydrolysis, aminolysis of esters, amide hydrolysis.

Unit-VI

7L

Elimination Reactions: E2, E1, Ecb Mechanisms, Orientation, stereochemistry in elimination, reactivity effect of structure attacking and leaving groups, competition between substitution & elimination, Saytzeff and Hoffman rules, Dehydration of Alcohols, Elimination not involving C-H Bonds, Pyrolytic eliminations, syn eliminations.

Reference Books

1. Frontier Orbitals and Organic Chemical Reactions, I. Fleming, 2nd ed. Wiley, New York 2004.
2. Reactive Intermediates in Organic chemistry, N. S. Issacs, John Wiley 1975.
3. R. T. Morrison and R. N. Boyd, Organic Chemistry, 6th ed., Prentice-Hall, 1992.
4. Jerry March, Advanced Organic Chemistry Reactions, Mechanism and Structure, 6th ed., John Wiley 2007.

5. S. M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry, 3rd ed. Macmillan, 2013
6. Peter Sykes, A Guidebook to Mechanism in Organic Chemistry Pearson, 2003

CH407: CHARACTERIZATION TECHNIQUES-I (Credits: 04, Lectures: 60)

Unit-I 3L

Presentation of Analytical Data: Accuracy, precision, classification of errors, significant figures, Mean deviation and standard deviation, treatment of small sets of data – Student T test and F test.

UNIT-II 12L

Separation Techniques: Chromatographic methods - principles, classification – Column chromatography, Liquid chromatography, Paper chromatography, HPLC, Thin layer chromatography, Ion-exchange chromatography, Gas chromatography, GC-mass chromatography.

UNIT-II 7 L

Ultraviolet and visible spectroscopy: Introduction, Beer Lambert's law, Morse potential energy curves, instrumentation, calculation of absorption maxima of dienes, dienones and polyenes, applications.

UNIT-III 7 L

Infrared Spectroscopy (IR): Introduction, instrumentation, sampling technique, selection rules, types of bonds, absorption of common functional groups. Factors affecting frequencies, applications.

UNIT-IV 15L

Nuclear Magnetic Resonance (NMR): Magnetic and nonmagnetic nuclei, Larmor frequency, absorption of radio frequency. Instrumentation (FT-NMR). Sample preparation, chemical shift, anisotropic effect, spin-spin coupling, coupling constant, Double resonance technique, applications to simple structural problems.

UNIT-V 16L

Mass spectroscopy (MS): Principle, working of mass spectrometer (double beam). Formation of different types of ions, McLafferty rearrangements, Nitrogen rule fragmentation of alkanes, alkenes, alkyl aromatics, alcohols and ketones, simple applications,

Reference Books

1. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch Fundamentals of Analytical Chemistry, 8th ed., Thomson Brooks/Cole Pub., Singapore. 2004.
2. H.H. Willard, L.L. Merritt, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, 7th ed., CBS Pub. New Delhi Reprint, 2004.
3. Vogels Textbook of Quantitative Chemical Analysis, Revised by G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney. ELBS, Longman, Essex U. K, 5th edn. (1996)
4. G. D. Christian, Analytical Chemistry, 5th ed, John Wiley & Sons, New York, 1994.
5. J. H. Kennedy, Principles of Analytical Chemistry, 2nd ed., Saunders Holt, London, 1990.

CH409: CHEMISTRY LABORATORY-I

(Credits: 03, Lectures: 60)

1. Mixture Analysis

2. Inorganic Preparations:

- (a) Tetraamine copper (II) sulphate monohydrate
- (b) Tris(Thiourea) copper(I) sulphate
- (c) Potassium trioxalato chromate (III) trihydrate
- (d) Hexaamine nickel (II) chloride

3. Organic Synthesis:

- (a) Synthesize an ester from its corresponding acid and alcohol (Fischer esterification).
- (b) Synthesis of Methyl salicylate (oil of wintergreen).
- (c) Synthesis of phthalimide (imide formation).
- (d) Synthesis of meta – nitro aniline (selective reduction).
- (e) Synthesis of anthracene maleic anhydride adduct (Diels – Alder Reaction.)
- (f) Synthesis of 7- hydroxy– 4 – methyl coumarin(Pechmann reaction).
- (g) Photoreduction of Benzpinacol.
- (h) To carry out photodimerisation reaction using maleic anhydride.
- (i) To synthesise a diagnostic agent (Flourescein).
- (j) Acetylation of primary amine (Preparation of acetanilide).
- (k) Base catalyzed aldol condensation (Synthesis of dibenzalpropanone).
- (l) Separate the components present in the given mixture by means of TLC.

- (m) Solvent-free reaction (Microwave-assisted ammonium formate-mediated Knoevenagel reaction).
- (n) Synthesis of p-benzoylpropionic acid from succinic anhydride and benzene (Friedal-Crafts reaction).
- (o) Synthesize and Characterize Methyl Orange Dye.

CH411: CHEMISTRY LABORATORY-II

(Credits: 03, Lectures: 60)

Kinetics

1. (a) To calculate specific rate constant k for acid catalyzed hydrolysis reaction of ethyl acetate at room temp.
(b) Energy of activation by measuring rate constant at two different temperatures.
2. (a) Study the kinetics of the reaction between potassium persulphate & KI. Determination of the rate const. & order of reaction.
(b) Study the influence of ionic strength on the rate constant.
3. Study saponification of ethyl acetate by sodium hydroxide solution using same initial concentration of both the reactants.
4. Study saponification of ethyl acetate by sodium hydroxide solution taking the initial concentration of ester and base to be different.
5. Studies kinetics of reaction between hydrogen peroxide and hydriodic acid.
(a) Determination of the rate constant (b) determination of activation energy.

Conductometry

6. Study precipitation titration between KCl and AgNO₃ conductometrically. Determine the strength of given solution of AgNO₃.
7. Determination of the solubility of barium sulphate by conductometry.
8. Determination of E_a of saponification of ester by conductometry method.
9. Estimation of the amount of acids present in a given mixture conductometrically.

Titrimetry and Separation technique

10. Paper chromatographic separation of Ni(III), Co(II) and Zn(II) ions.
11. Study precipitation titration between KCl and AgNO₃. Determine the strength of given solution of AgNO₃.
12. Determination of copper by complexometric titration.

13. Determine the strength of given potassium dichromate solution with N/20 hypo solution
14. Interpretation of IR spectrum.
15. Interpretation of NMR spectrum with reference to calculation of chemical shift.

Reference books:

1. Text Book of Vogel's Practical Organic Chemistry by Longman Group, B.S. Furness et. al., Ltd.
2. Louis F. Fieser "Experiments in Organic Chemistry", 2nd ed. D.C. Heath and Company Boston, 1955.
3. "Organic Synthesis" Collective Vol. I. Caltexas, 2012
4. R.K. Bansal, Laboratory Manual in Organic Chemistry, Wiley Eastern Ltd., New Delhi, 1980.
5. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch Fundamentals of Analytical Chemistry, 8th ed., Thomson Brooks/Cole Pub., Singapore. 2004.

Semester II

CH402: PHYSICAL CHEMISTRY – II

(Credits: 04, Lectures: 60)

Unit I

18L

Surface chemistry and catalysis: Surface tension and surface free energy; Pressure across an interface: Laplace equation, Kelvin equation; Wetting: Young-Dupre equation.

Adsorption in liquid systems: Gibbs adsorption isotherm; Adsorption on solids: Langmuir isotherm, BET isotherm, transition state theory of surface reactions: rates of chemisorption and desorption, unimolecular and bimolecular surface reactions. Micelles-Surface active agents and their classification, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, thermodynamics of micellization-phase separation and mass action models, micro emulsions, reverse micelles. Heterogeneous catalysis, surface heterogeneity, surface catalyzed unimolecular and bimolecular reactions, temporary and permanent catalytic poisons, activation energy for surface reactions. Comparison of uncatalyzed and catalyzed reaction rates.

Unit-II

15L

Quantum Mechanics: The postulates of quantum mechanics, Linear and Hermitian operators. Commutation of operators and Uncertainty Principle. Schrödinger equation, eigen function and eigen values, free particle, Schrödinger equation for a particle in a box, the degeneracy, particle in a box with a finite barrier, Schrödinger equation for linear harmonic oscillator and its solution, zeropoint energy.

Unit III

12L

Photochemistry: Absorption of light and nature of electronic spectra, electronic transition and intensity of absorption bands, Frank-Condon principle, construction of Jablonski diagram, photophysical pathways of excited molecular system (radiative and non-radiative), Quenching and Stern-Volmer equation. Kinetics of photochemical reactions.

Unit IV

15L

Phase Equilibria: Statement and meaning of the terms in Gibbs phase rule; Thermodynamic derivation of Gibb's phase rule, phase equilibria of Water, Helium and Carbon systems; Two component solid-liquid equilibria (example of Cu-Ni alloy): simple eutectic; congruent

melting type; peritectic type and monotectic type phase diagrams, concept of Phase equilibria of three component systems, Applications of phase equilibrium.

Reference books:

1. S. Glasstone- Text book of Physical Chemistry 1936.
2. G. M. Barrow –, Physical Chemistry Tata-McGraw Hill, Vth edition, 2003.
3. R. Stephen Berry, Stuart A. Rice and John Ross, Physical Chemistry 2nd edn, Oxford Univ. Press, New York, 2000
4. J.I. Steinfeld, J.S. Francisco and W.L. Hase, Chemical Kinetics and Dynamics, 2nd edn, Prentice Hall, New Jersey, 1999.
5. P. W. Atkins, and Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
6. D. A. Mc Quarrie and D. Simon, Physical chemistry, A Molecular Approach ,Viva Books Pvt. Ltd, New Delhi, 2003.
7. D. A. Mc Quarrie, J. D. Simon, Molecular Thermodynamics, University Science Books, Sausalito, California, 1999.
8. Horia Metiu, Physical Chemistry, Thermodynamics Taylor & Francis, 2006.
9. R. J.Silbey, , R. A. Alberty, & M. G. Bawendi, Physical Chemistry 4th Ed. Wiley ,2004.
10. Physical Chemistry by Walter J Moore, Published by Prentice-Hall, 1983

CH404: INORGANIC CHEMISTRY-II

(Credits: 04, Lectures: 60)

Unit I

15L

Coordination Chemistry: Spectra and Magnetism-I: Coupling of Angular Momenta (Spin-Spin Coupling, Orbital-Orbital Coupling and Spin-Orbital Coupling), Energy Terms Symbols and their Derivations using Vector Diagrams, Calculation of L,S,and J term symbols, Determination of Ground State Terms-Hund's rules, Hole Formalism, Microstate and their Calculations, Spin-Orbital Coupling Parameter.

Unit II

20L

Coordination Chemistry: Spectra and Magnetism-II: Electronic Spectra, Selection Rules and their Relaxation, Interpretation of Electronic Spectra, Orgel and Tanabe-Sugano Diagrams, Nephelauxetic Effect, Calculations of $10 Dq$, Racah Parameters B and β and

Transition Energy, Charge Transfer Spectra, Magnetic Properties of Metal Complexes, Types of Magnetisms, Calculations of Magnetic Moments, Anomalous Magnetic Moments-Quenching of Angular Momentum.

Unit III **10L**

Metal Clusters: Higher Boranes, Borazine, Carboranes, Metalloboranes and Metallocarboranes, Halide and Carbonyl Clusters.

Unit IV **15L**

Metal Pi-Complexes: Metal Carbonyls: Preparation, Reactions, Structure and Bonding, Vibrational Spectra of Metal Carbonyls for Bonding and Structural Elucidation, Preparation, Bonding, Structure and Reactions of Transition Metal Nitrosyl, Dinitrogen and Dioxygen Complexes, Tertiary Phosphine as Ligand.

Reference Books:

1. J. D. Lee, Concise Inorganic Chemistry, 5th ed., Elbs with Chapman and Hall, London 2008.
2. J.N.Murre, SFA Kettle and JM. Tedder, The Chemical bond, 2nd ed. Wiley, New York 1996.
3. F.A. Cotton and Wilkinson, Advanced Inorganic Chemistry, 6th ed. John Wiley 2006.
4. J.E. Huhey, Inorganic Chemistry, 4rd ed. Harper & Row, New York, 2006.
5. T. Moeller, Inorganic Chemistry, A Modern Introduction, John Wiley and Sons 1985.
6. Chemical application and Group theory, 3rd edition F.A. Cotton 2008.

CH406: ORGANIC CHEMISTRY-II

(Credits: 04, Lectures: 60)

Unit-I **15L**

Stereochemistry-I: Symmetry elements, D-L, R-S, E-Z and threo-erythro nomenclature, interconversion of Fischer, Newman, Sawhorse and flying wedge formulae. Conformational analysis, enantiomerism and diastereomerism of simple, cyclic (chair and boat configuration) and acyclic systems. Axial and planer chirality, optical isomerism in allenes, biphenyls (atropoisomerism), spiranes, hemispiranes. Elementary ideas about stereochemistry of tertiary amines, quaternary salts, sulphur and phosphorous compounds.

Unit-II **15L**

Stereochemistry-II: Topicity of ligands and faces, their nomenclature and prostereoisomerism, stereogenecity, chirogenicity, pseudoasymmetry and prochiral centre.

stereospecific and stereoselective reaction. Stereochemistry of sugars- C1 and 1C conformations of hexoses, c2'-endo and c3'-endo conformation of pentoses. Chemical correlation of configuration-determination of relative configuration of 2-butanol, isoserine, alanine, malic acid, lactic acid and mandelic acid.

Unit-IV

15L

Pericyclic Reactions I: Molecular orbital symmetry, frontier orbital of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system classification of pericyclic reactions, Woodward- Hoffmann correlation diagram. FMO & PMO approach, Electrocyclic reaction - conrotatory and disrotatory motions. $4n$, $4n+2$, allyl systems, Ring opening of cyclopropyl halides and tosylates, cycloadditions-antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, $2+2$ addition of ketenes, 1,3-dipolar cycloadditions and cheletropic Reactions.

Unit V

15L

Pericyclic Reactions II: Sigmatropic Rearrangements-suprafacial and entarafacial shifts of H, sigmatropic shifts involving carbon moieties, retention and inversion of configuration, [3, 3] and [5, 5] sigmatropic rearrangements, detailed treatment of Sommelet-Hauser, Claisen and Cope rearrangement's introduction to ene reactions. Simple problems on Pericyclic reactions, Group transfers and eliminations.

Reference Books

1. Fleming, Frontier Orbitals and Organic Chemical Reactions, 2nded.Wiley, New York 2004.
2. P. S. Kalsi, Stereochemistry, 5th ed., New Age International 2010.
3. R. T. Morrison and R. N. Boyd, Organic Chemistry, 6th ed., Prentice-Hall, 1992.
4. Jerry March, Advanced Organic Chemistry Reactions, Mechanism and Structure, 6th ed., John Wiley 2007.
5. S. M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry, 3rd ed. Macmillan, 2013.

UNIT I:**10L**

Introduction, Concept and need of Green Chemistry in our day-to-day life, Development of Green Chemistry, Green Chemistry and sustainability, Dimensions of sustainability, Limitations/Obstacles in pursuit of the goals of Green Chemistry, Opportunities for the next generation of materials designers to create a safer future.

UNIT II:**15L**

Basic principles of Green Chemistry- (i) Prevention of waste/byproducts. (ii) Maximum Incorporation of the materials used in the process into the final product (Atom Economy): Green metrics (iii) Prevention/Minimization of hazardous/toxic products (iv) Designing safer chemicals - different basic approaches (v) Selection of appropriate auxiliary substances (solvents, separation agents etc) (vi) Energy requirements for reactions-use of microwave, ultrasonic energy (vii) Selection of starting materials-use of renewable starting materials (viii) Avoidance of unnecessary derivatization-careful use of blocking/protection groups, (ix) Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents. (x) Designing biodegradable products. (xi) Prevention of chemical accidents. (xii) Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

UNIT III: Green energy sources for chemical synthesis.**5L****Reference Books:**

1. Green Chemistry: Theory and Practice. P.T. Anastas and J.C. Warner. Oxford University Press.
2. Green Chemistry: Introductory Text. M. Lancaster Royal Society of Chemistry (London).
3. Introduction to Green Chemistry. M.A. Ryan and M.Tinnesand, American Chemical Society (Washington).
4. V.K. Ahluwalia, Methods and Reagents of Green Chemistry: An Introduction by Green Chemistry

1. Inorganic Preparations:

- (a) Bis(dimethylglyoximate) nickel (II)
- (b) Hexaamine cobalt (III) chloride
- (c) Hexaamine cobalt (III) hexanitritocobaltate
- (d) Ammonium diamminetetra-thiocyanato chromate

2. Separation and estimation of two metal ions

- (a) Copper-Nickel
- (b) Barium-Copper
- (c) Copper-Zinc
- (d) Nickel-Zinc
- (e) Copper-Iron
- (f) Iron-Nickel
- (g) Copper-Magnesium
- (h) Lead-Copper
- (i) Calcium-Magnesium
- (j) Zinc-Magnesium

(A) Organic Synthesis

1. [4+2] cycloaddition reaction (Diels-Alder reaction between furan and maleic acid)
2. To prepare benzoic acid from benzyl using green approach (Benzil-Benzoic acid rearrangement).
3. Electrophilic aromatic substitution reaction-i (Nitration of phenol)
4. Pinacolpinacolone rearrangement reaction (Preparation benzopinacolone)
5. Radical coupling reaction (Preparation of 1, 1'-bis-2-naphthol).
6. Transesterification reaction (Synthesis of biodiesel)
7. Acetylation – preparation of acetanilide from aniline
8. Preparation of hippuric acid (N-Benzoylation)

(B) Multi - step synthesis of organic compounds

1. Synthesis of 2-phenyl indole (Fischer Indole synthesis)
2. Synthesis of benzanilide (Beckmann rearrangement)
3. Synthesis of sulphanilamide

(C) Estimation of drugs: Aspirin and Ibuprofen

(D) Microwave Assisted Organic Synthesis: Hydrolysis of benzamide by using Microwave Irradiation Technique

(E) To deduce the structure of organic compounds from the given spectral data (IR & NMR)

1. Phase Equilibria

- i. Determination of the critical solvent temperature of phenol & water in the 1.0 % NaCl
1.0 % Succinic acid
- ii. Determination of congruent composition & temperature of binary system diphenylamine
& benzophenone.
- iii. Determination of the Phase Diagram for ethyl acetate, ethyl alcohol and water system
(Three component system).
- iv. Determination of the Phase Diagram for Benzene, ethyl alcohol and water system (Three
component system).

2. Surface Chemistry

- i. Study the variation of the surface tension of n-propyl alcohol with concentration by the
help of stalagmometer.
- ii. Comparison of cleaning power of given different samples of detergent.
- iii. Study adsorption of a solute (oxalic acid/acetic acid) by activated charcoal from an
aqueous solution.

3. Spectral Techniques

- i. Calculation of λ max of the given sample using UV-Vis spectrophotometer.
 - i. Determination concentration of sulphate spectrophotometrically.
 - ii. Determination concentration of phosphate spectrophotometrically.
- iii. Soft lab on FTIR

Reference books

1. Text Book of Vogel's Practical Organic Chemistry by Longman Group, B.S. Furness et
al., Ltd.
2. Louis F. Fieser "Experiments in Organic Chemistry", 2nd ed. D.C. Heath and Company
Boston, 1955.
3. "Organic Synthesis" Collective Vol. I. Caltexas, 2012
4. R.K. Bansal, Laboratory Manual in Organic Chemistry, Wiley Eastern Ltd., New Delhi-
1980.
5. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch Fundamentals of Analytical
Chemistry, 8th ed., Thomson Brooks/Cole Pub., Singapore. 2004.

CH414: COMPUTATIONAL METHODS IN CHEMISTRY

(Credits: 02, Lectures: 30)

1. Introduction: Computational chemistry and its applications: History, Accuracy, Methods and Fields of application.

2. In-silico drug design: Methods used in in-silico drug design Homology modeling Molecular docking (Interaction networks), In silico Chemical Libraries, Virtual high-throughput screening, Active site directed Drug Design, Ligand and Structure Based Drug Design.

3. Chemical Drawing: Three-Dimensional Effects, Optical Activity, Computer Packages, Modelling, Molecular Structure database, File formats, Three Dimensional Displays, Proteins, Introduction to chemi-informatics.

4. Hands on exercise: Structural Drawing using Chems sketch and ChemDraw softwares, study of their Physiochemical and spectral properties.

5. Modeling Exercise: Visualization of 3D structure of proteins, identification of pocket, solvent accessibility, co-ordinates, surface, RMSD etc.

6. Web based tools: Introduction to online drug designing/modeling software's, online molecular libraries, similarity search analysis using following

- ChemMine Tool: similarity Search Analysis
- Discovery Gate similarity Search Analysis
- Basespace: correlation soft ware
- Collaborative Drug Discovery (CDD)
- ChEMBL
- Discovery Gate

Reference Books:

1. Essentials of Computational Chemistry: Theories and Models by Christopher J. Cramer, Publisher: Wiley (first edition).
2. Molecular Modelling: Principles and Applications (2nd Edition) by Andrew R. Leach, Publisher: Prentice Hall (second edition).
3. Introduction to Computational Chemistry by Frank Jensen, Publisher: Wiley (first edition).
4. Molecular Modelling for Beginners by Alan Hinchliffe, UMIST, Manchester, UK, Wiley

Discipline Specific Elective-I (Select any one)

CH 416: MEDICINAL CHEMISTRY-I

(Credits: 03, Lectures: 45)

Unit I

5L

Introduction to Drug action and metabolism: ADME (Absorption, Distribution, Metabolism and Elimination of Drugs), Bioavailability of drugs, Lipinsky rule of five, Prodrugs and Soft Drugs, Drug Resistance and Drug Synergism, concept of LD₅₀ ED₅₀ and Therapeutic Index.

Unit-II

10L

Drug Discovery, Drug Design and Development: History of development of chemotherapeutic agents, Various approaches of Drug Discovery and Development, naming of (new) drugs, Procedure followed for lead discovery (rational and random approaches), Lead optimization, Molecular Modification of Lead Compound, Structure-Activity Relationship (SAR).

Unit-III

10L

Quantitative Structure Activity Relationship (QSAR)L: Physicochemical parameters, electronic effects; Hammett Equation, Lipophilicity Effects; the lipophilicity substituents constant, Log P calculation and significance in bioavailability of drugs; Hansch Equation, Steric Effects; The Taft Equation, Methods used to correlate Physicochemical Parameter with Biological Activity; Hansch analysis, Craig Plot, Free and Wilson Analysis, Topliss operational scheme.

Unit IV

10L

Drug Receptor Interaction: Receptors and Receptors structure, Determination of Drug Receptor Interaction by dose response curve and concept of Agonist and Antagonist, Forces involved in the Drug-Receptor Complex formation, Drug Receptor Theories; Occupancy theory, Rate theory, Induced-Fit theory.

UnitV

10L

Combinatorial Chemistry: Introduction to Combinatorial approaches, Combinatorial libraries/Chemical Diversity, Impact of Combinatorial Libraries in Drug discovery process, Combinatorial Synthesis and testing methods; solid phase synthesis, combinatorial mixtures, mixed building block strategy, High Throughput Screening (HTS).

Reference Books:

1. Burger's Medicinal Chemistry and Drug Discovery Vol-I 6th ed. M.E. Wolf, John Wiley, 2003.
2. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill, 2014.
3. Text book of Synthetic Drugs, Gurdeep R. Chatwal, Himalaya Publication House, 2013.
4. Text book of Medicinal Chemistry by Madhu Chopra V. K. Ahluwalia, Publisher; Ane Books Pvt. Ltd.2010
5. Essentials of Medical Pharmacology by K. D. Tripathi, Jaypee Brothers Medical Publishers (P) Ltd, 2008.
6. Essentials of Medicinal Chemistry by Andrejus Korolkovas, Second Edition, A wiley-Inter-science Publication, New York, 2008.

CH 418: BIOMOLECULES

(Credits: 03, Lectures: 45)

UNIT-I

14L

Carbohydrates-Structure and biological functions of important monosachharides (excluding detailed conformational analysis) and derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars-N-acetylmuramic acid and sialic acid. Disaccharides- sucrose, lactose and maltose.

Structure and biological functions of Structural polysaccharides (cellulose and chitin) and Storage polysaccharides (starch and glycogen) Heteropolysaccharides- glucosaminoglycans/mucopolysaccharides. Glycoconjugates- glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances.

UNIT-II

7L

Lipids-Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids

Lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure.

UNIT-III

8L

Amino-acids, Peptides and Protein- Peptide bond, Chemical and enzymatic hydrolysis of proteins to peptides, Sanger method and Edman degradation method for amino acid sequencing. Secondary structure of proteins- α -helix, β -sheet, forces responsible for holding the secondary structures of proteins.

UNIT-IV**8L**

DNA and DNA- Interactive Agents-Introduction: Basis for DNA-interactive drugs, Toxicity of DNA-interactive drugs, Classes of drugs that interact with DNA:

UNIT-V**8L**

Steroids and Hormons: Isolation and nomenclature of steroids. Structure elucidation, synthesis (Woodward) and stereochemistry of cholesterol.

Methods for the following conversions.

- i) Cholesterol → Testosterone
- ii) Cholesterol → Progesterone
- iii) Cholesterol → 5- α and 5- β cholanic acids.

Johnson's hydrochrysene approach towards the synthesis of Androsterone.

Introduction to steroidal and non steroidal Hormones

Reference Books:

1. Organic Chemistry, Vol 2, I. L. Finar, ELBS, 2002.
2. K Anand Solomon, Chemistry of Natural Products, MJP Publishers, 2012
3. Bhimsen A. Nagasampagi, Meenakshi Sivakumar, and Sujata V. Bhat, Chemistry of Natural Products, Springer, 2005.
4. Alagarsamy, Pharmaceutical Chemistry of Natural Products, 2012
5. Text book of Medicinal Chemistry by Madhu Chopra V. K. Ahluwalia, Publisher; Ane Books Pvt. Ltd. 2010

CH420: POLYMER CHEMISTRY-I**(Credits: 03, Lectures:****UNIT-I****8L**

Introduction: Defining Polymers, Classification of Polymers, Bonding in Polymers, Copolymers, and Why Polymers are different from small molecules

UNIT-II**15L**

Chain Growth Polymerization: Addition Polymerization, Free radical addition, Non-radical Addition Polymerization, Cationic Polymerization, Anionic Polymerization, Heterogeneous Stereospecific Polymerization, Ziegler - Natta polymerization, Metallocene Polymerization, Olefin Metathesis, Kinetics of cationic, anionic and free radical polymerization

UNIT-III**12L**

Step Growth Polymerization: Condensation Polymerization, Noncondensation Polymerization, Functionality Principle and Relationship between average functionality, extent of reaction and degree of polymerization (X_n), Kinetics.

UNIT-IV**10L**

Copolymerization: Growth copolymerization, Free Radical Copolymerization, Step growth copolymerization, Ionomers, Polymer blends and interpenetrating polymer networks, Utility of copolymerization.

Reference Books

1. F.W. Billmeyer, Jr. Textbook of polymer science, Wiley- Interscience, N.Y. 1971.
2. R. Seymour, Introduction to polymer chemistry, Wiley –Interscience, 1981.
3. D.D. Deshpande, Physical chemistry of Macromolecules, Vishal publications, 1985.
4. P.J. Flory, Principles of polymer chemistry, Cornell University Press, 1953.
5. V R Gowarikar, Polymer Science, New Age International Pvt Ltd Publishers, 2010.
6. G.Odian, Principles of polymerization, 4th ed. Wiley – Interscience 2004.
7. Condensation polymers by interfacial and solution methods, Paul W. Morgen, Interscience publishers

CH422: BIOINORGANIC CHEMISTRY-I**(Credits: 03, Lectures: 45)****Unit I****8L**

Introduction, Metal function in Metalloproteins, Functions of Metalloenzymes, Communication roles for metals in Biology, Interactions of metal ions and nucleic acids, Metal-Ion Transport and Storage, General aspects of storage and transport of metal-ions- Iron, Calcium, Copper, Metals in medicines. Metal ions in Biological Systems-Metal ions: Their excess and deficiency (Ca, Mg, K, Na, Co, Zn, Mo, Cr, Cu, Fe)

Unit II**8L**

Essential and Trace Metals-Criteria for essential elements, Essential ultratrace elements, essential ultratrace Non metals, toxicity and deficiency, toxic effects of trace elements: Pb, Ar, Cd, Hg, Cu, Zn.

Unit III **16L**

Role of metal ions in Biological Systems (I)-Non-protein Metallobiomolecules–Photoredox, Non-protein Metal transport and structural Metallobiomolecules, The bacterial Iron transport, Proteins–Transport and Storage Protein metallobiomolecules, Electron Carriers, Metal Storage and structural metallobiomolecules, Oxygen binding metallobiomolecules, Protein-Enzyme Metallobiomolecules. Metal ions in biological systems: Na, K, Li, Ca, Mn, Zn, Cu

Unit IV **7L**

Structure and functions of cell membrane, Ion transport through cell membrane and Na^+/K^+ pump: Passive mediated transport, Active Transport, Na^+-K^+ -ATPase, Ca^{2+} -ATPase, ABC transporters, Sodium potassium pump

Unit V **6L**

Chlorophyll- Simple reactions of chlorophyll, Extraction of chlorophyll from plants, Health Benefits of chlorophyll. Porphyrin-containing compounds: Haemoglobin and Myoglobin

Reference Books:

1. Bioinorganic chemistry -Bertini Ivano, Gray H. B., Lippard S. J. & Valentine J. S. University Science Books Mill Valley, California. ISBN 0-935702-57-1.
2. Principles of Bioinorganic chemistry - S. J Lippard & M. J. Berg (1997).
3. Inorganic Biochemistry, (Vol.I & II) - G. L. Eicchor. Bioinorganic chemistry. A. K. Das. Books & Allied (P) Ltd.
4. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life. Wolfgang Kaim and Brigitte Schwederski (2012)
5. Concepts and Applied Principles of Bioinorganic Chemistry: Volume II: 2 Warren Gibbs (2015).
6. Concepts and Applied Principles of Bioinorganic Chemistry: Volume III: 3 Warren Gibbs (2015).
7. An introduction to bio-inorganic chemistry. Williams, D R (2016)
8. Bioinorganic Chemistry : Dieter Rehder and Ebbe Nordlande (2014)

Semester III

CH 503: Green Chemistry-II

(Credits: 03, Lectures: 45)

Unit-I: Introduction to green starting materials, green reagents, Green solvents and reaction conditions. **5L**

Unit II: Green solvents: Aqueous medium- Enhancement of selectivity, efficiency, and industrial applicability; Ionic liquids; Supercritical fluids; Solvent free neat reactions in liquid phase; Solvent free solid phase reactions; Fluorous phase reactions. **10L**

Unit III: Some examples of Microwave assisted reaction; Ultrasound assisted reactions; Photochemical reactions, Electrochemical synthesis. **10L**

Unit IV: Green catalysis: Heterogeneous catalysis- Use of zeolites, silica, alumina, clay, polymers, cyclodextrin, and supported catalysts, Phase-transfer catalysis (micellar/ surfactant etc) **10L**

UNIT V: Industrial Case Studies: Methyl Methacrylate (MMA); Greening of Acetic acid manufacture; Vitamin C; Leather manufacture- Hide and Skin-Tanning, Reverse tanning, Vegetable tanning, Chrome tanning; Fat liquoring; Dyeing; Eco friendly Pesticides and Insecticides. **10L**

Reference books:

1. Introduction to Green Chemistry, M.A. Ryan and M.Tinnesand, American Chemical Society (Washington), 2003.
2. Real World Cases in Green Chemistry (Vol 1), M.C. Cann and M.E. Connelly. American Chemical Society (Washington). Product code: 206-105.
3. Real World Cases in Green Chemistry (Vol 2), M.C. Cann and T.P.Umile. American Chemical Society (Washington), Product code: 206-113.
4. Alternative Solvents for Green Chemistry, F.M. Kerton, Royal Society of Chemistry (London), 2013.
5. Recoverable and Recyclable Catalysts, M. Benaglia, Wiley, 2009.
6. Handbook of Green Chemistry & Technology. J. Clark and D. Macquarrie, Wiley Publishing, 2007.
7. Solid-Phase Organic Synthesis. K. Burgess. Wiley-Interscience, 2002.
8. Eco-Friendly Synthesis of Fine Chemicals. R. Ballini. Royal Society of Chemistry, 2009

CH 505: PATENT LAWS AND IPR ISSUES**(Credits: 02, Lectures: 30)****UNIT-I****4L**

Drug & Cosmetics Act with special reference to schedule Y and M, schedule of medical devices.

UNIT-II**8L**

Concept of total quality management, requirements of GMP, GLP, GCP, Regulatory requirements of drugs and Pharmaceutical (USFD-NDA/ ANDA)

UNIT-III**8L**

Documentation and Maintenance of records.

UNIT-IV**6L**

Intellectual property rights patents, Trademarks, Copyrights, Patents Act.

UNIT-V**4L**

Environment protection Act, Pollution Control, Factories Act.

Reference Books

1. Willing, S.W., & Stoker, Good Manufacturing Practices for Pharmaceuticals, Marcel Dekker, New York.
2. Guarino, R.A., New Drug Approval Process, Marcel Dekker, New York.
3. Drug & Cosmetic Act.
4. Patents Act.
5. Consumer Protection Act.
6. Environmental Protection Act.
7. Federal Food, Drug & Cosmetic Act.
8. Bansol, IPR Guidelines for Pharm students and Researchers.
9. Pisano-FDA Regulatory Affairs.
10. Phillip W. Grubb, Patents for Chemicals, Pharmaceuticals and Biotechnology

Discipline Specific Electives (DSE-II) (Select any one)

CH 511: MEDICINAL CHEMISTRY-II

(Credits: 03, Lectures: 45)

Synthesis, General Mode of Action and Medicinal Uses of Important Drugs in the Following Categories;

Unit I **10L**

Drugs Affecting Central Nervous System: Sedative, Hypotonic and Anticonvulsant; Alcohols, Aldehydes, Ketones, Sulphones, Urethanes, Amides, Ureas, Barbiturates and Hydantoin. Synthesis of Carbromal, Veronal and luminal.

Tranquillizers; Rauwolfia alkaloids, Phenothiazine, Thioxanthene, Butyrophenone and Indole derivatives. Synthesis of Chlorpromazine and Haldol.

CNS Stimulants and antidepressant drugs; Analeptics, Purines, Iminodibenzyls

Unit II **10L**

Drugs Affecting Autonomic Nervous System: Cholinergic and anticholinergic Agents; Esters of Choline, Cholinomimetic alkaloids, anticholinesterases.

Adrenergic stimulant & Blocking agent; Aliphatic amines, Epinephrine and related compounds (dopamine). Blocking agents; Ergot alkaloids and Imidazolines.

Anaesthetics; Classification, Natural, Volatile and Nonvolatile anaesthetics, Local and General Anaesthetics (LA and GA).

Histamine & anti-histaminic agents; Diaryl-carbinyl Ethers, Diarylalkylenediamines Phenothiazine and propylamine derivatives.

Unit III **10L**

Drugs affecting Cardiovascular System: Cardiotonic drugs/cardiac glycosides, Anti-anginal agents, Calcium Channel Blockers, β -blockers, Antiarrhythmic agents, Antihypertensive drugs: ACE inhibitors and Vasodilators, Antihypercholesterolemic agents, Sclerosing agents.

Unit IV **05L**

Diuretics: Introduction, Classification of Diuretics, Mercural and Osmotic diuretic agents, Carbonic Anhydrase Inhibitors, Thiazides and Hydrothiazide and High Ceiling Diuretics,

Unit V **10L**

Antipyretics Analgesics and Anti-inflammatory Drugs: Introduction of Antipyretics and Analgesics, Classification of analgesics; Pyrazolone and Pyrazolidones, Aniline, p-

aminophenol derivatives, Quinoline derivative, Morphine and related compounds. Aanti-inflammatory drugs, Salicylic acid derivatives and N-aryl anthranilic acid derivatives.

Reference Books:

1. Burger's Medicinal Chemistry and Drug Discovery Vol-I 6th ed. M.E.Wolf, John Wiley, 2003.
2. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill, 2014.
3. Text book of Synthetic Drugs, Gurdeep R. Chatwal, Himalaya Publication House, 2013.
4. Text book of Medicinal Chemistry by Madhu Chopra V. K. Ahluwalia, Publisher; Ane Books Pvt. Ltd.2010
5. Essentials of Medical Pharmacology by K. D. Tripathi, Jaypee Brothers Medical Publishers (P) Ltd, 2008.
6. Essentials of Medicinal Chemistry by Andrejus Korolkovas, Second Edition, A wiley-Inter-science Publication, New York, 2008.

CH 513: BIOINORGANIC CHEMISTRY-II

(Credits: 03, Lectures: 45)

Unit-I

12L

Metal ions in carcinogenesis:

General and biochemical aspects of cancer, carcinogens and anticancer agents. Carcinogenesis

and its mechanism. Role of metal complexes and Pt(II) and (IV) as anticancer agents anticancer activity of rhodium, gold, copper, and cobalt complexes. Selenium and its biochemical role and its mechanism of cacinostatic actions. Some representative metallodrugs containing arsenic, antimony, gold, mercury and tin metal. Antibacterial, antifungal and antiviral activity of metal; complexes.

Unit- II

12L

Concepts on metal ion toxicity: Metal ion toxicity in man and animals. Introduction, general aspects of Pb(II), Cd(II), and Hg(II),biochemical and physiological effects caused due to Pb(II), Cd(II), and Hg(II) ion toxicity.Detoxifications of these metals using chelating agents.

Unit-III**12L**

Interactions of metal ions and metal complexes: Structure and functions of amino acids, proteins, peptides, enzymes nucleoside, nucleotide and comparative study of structures and functions of these biomolecules. Metal ion binding sites present in amino acids, peptides, proteins, enzymes, nucleoside and nucleotide. Interactions of metal ion and metal complexes with these biomolecules.

Unit-IV**9L**

Metals in medicine: Chelation therapy, Limitation of chelation therapy in metal ion detoxification, Zinc salt in the treatment of sickle cell anemia. Lithium therapy in psychiatric mind disorder, Metals used in diagnosis, radiodiagnostic agent, MRI and X-ray contrast agent, Bismuth and Vanadium compound in medicines, chelation and role of metal complexes in conventional drug resistant malaria

Reference Books:

1. Pharmacological basis of therapeutic, 5th and 6th edition by –Louis S. Goodman, (Macmillan Publishing company, New York, Toronto and London)
2. Metal ions in biological system - Helmut Sigel. Vol. 19, 21, 22 - (Marcel Dekker INC, New York and Basel)
3. Metal ions in biological system (Concepts on metal ion toxicity) by Helmut Sigel. Vol.7-(Marcel Dekker INC, New York and Basel)
4. Bioinstrumentations – L Veerakumari , MJP publisher Chennai
5. Principles of bioinorganic chemistry – S. J Lippard & J M Berg , Mill Valley California
6. Elements of Bioinorganic - G N Mukherjee, and Arbinda Das U N Dhur and Sons Pvt. Ltd Kolkatta

CH515: POLYMER CHEMISTRY-II**(Credits: 03, Lectures: 45)****UNIT-I****7L**

Polymer Properties: Structure-property relationship, Average Molecular Weight, Polydispersity index, Effect of Polymerization Mechanism on PDI

UNIT-II**10L**

Polymer solutions and solubility: Polymer solutions and solubility, Dissolution of Polymers, General Rules for Polymer Solubility, Thermodynamic basis of polymer-solubility, thermodynamic basis of polymer-solubility, Solubility Parameters, Properties of dilute sol

UNIT-III**10L**

Solid State Properties: Amorphous State, Crystalline State, Requirements for Crystallinity, Deformations in polymers, Flow Behavior, Purely Viscous Flow, Time-dependent behavior, Polymer Melts and Solutions, Transitions in Polymers, Molecular Motions in Polymers, Determination of T_g

UNIT-V**8L**

Polymerization Practice: Bulk Polymerization, Solution Polymerization, Emulsion Polymerization, Suspension Polymerization, Interfacial Polycondensation

UNIT-VI**10L**

Polymer Processing: Introduction, Basic Processing Operations, Extrusion, Calendering, Stamping, Casting, Solution Casting, Blow Molding, Spinning

Reference Books

1. Mayo Smith, Polymer Production, Reinhold Pub. Corp., 1958
2. L.H. Peebles, Molecular weight distribution in polymer, Wiley- Interscience, N.Y. 1971
3. H. Morawetz, Macromolecules in solution, Wiley Interscience, N.Y. 1975.
4. E.A. Turi, Thermal characterization of polymeric materials, Academic press Inc, 1981.
5. G.C. Levy and G.L Nelson Carbon-13 Nuclear Magnetic Resonance for organic chemists, Wiley Interscience, N.Y. 1980.
6. F.W. Billmeyer, Jr. Textbook of polymer science, Wiley- Interscience, N.Y. 1971.
7. B.R Gupta Polymer Processing Technology. Asian Books Private Limited, 2008

Discipline Specific Electives (DSE-III) (Select any one)

CH517: CATALYSIS

(Credits: 03, Lectures: 45)

Unit I

10L

Fundamentals: Catalyst - activation energy concept - types of catalysis - comparison of homogeneous & heterogeneous catalysis - enzyme catalysis - green catalysis - nano catalysis - autocatalysis - phase transfer catalysis - promoters - poisons - examples.

Unit II

10L

Heterogeneous catalysis: Adsorption isotherms - surface area - pore size and acid strength measurements - porous solids - catalysis by metals - semiconductors and solid acids - supported metal catalysts - catalyst preparation - deactivation and regeneration.

Unit III

15L

Characterization of solid catalysts: Surface area - structure - surface morphology – porosity - pore volume - diameter - particle size - X-ray diffraction - SEM, TEM, XPS and TPD, TPR for acidity and basicity of the catalysts.

Unit IV

10L

Photocatalysis: Generation of hydrogen by photo catalysts - photo catalytic break down of water and harnessing solar energy - photocatalytic degradation of dyes – environmental applications.

Reference Books:

1. P.H. Emmet, Catalysis (Vol I and II), Reinhold, New York, 1954.
2. M. Schlosser, Organometallics in Synthesis, A manual, John Wiley, New York, 1996.
3. L.S. Hegeudus, Transition Metals in the Synthesis of Complex Organic Molecules, University Science, Book, CA, 1999.
4. D.K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, New Age, 2008.
5. B. Viswanathan, S. Kannan, R.C. Deka, Catalysts and Surfaces: Characterization Techniques, Narosa, New Delhi, 2010.
6. M. Kaneko, I. Okura, Photocatalysis: Science and Technology, Springer, 2003.

CH519: CHARACTERIZATION TECHNIQUES-II**(Credits: 03, Lectures: 45)****Unit-I****15L**

Titrimetric Analysis: Acid-base titration – theory, indicators – mixed indicators, universal indicators, neutralization curves. Complexometric titrations – EDTA titrations – theory, indicators, applications – masking and demasking agents. Redox titration– Permanganometry & dichrometry. Iodimetry- theory. Precipitation titrations.

UNIT-II**15L**

Thermal Methods of Analysis: Introduction to thermal analysis, TG and DTG, Instrumentation, thermogram, factors affecting thermograms, application of thermogravimetry. Differential thermal analysis, DTA theories, DTA curves, factors affecting DTA curves, Instrumentation, applications of DTA, simultaneous determination in thermal analysis. Differential Scanning Calorimetry (DSC): Introduction, Instrumentation, DSC-curves, factors affecting DSC curves, applications.

UNIT-III**15L**

X-ray & neutron diffraction: a) Fundamentals of x-ray diffraction, Theory of x-ray diffraction, diffraction of x-rays by crystals, determination of crystal structure (powder as well as single crystals), Instrumentation, determination of lattice parameters, x-ray intensity calculations and application of x-rays

b) Introduction to neutron diffraction, theory, Instrumentation and application

Reference Books

1. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch Fundamentals of Analytical Chemistry, 8th ed., Thomson Brooks/Cole Pub., Singapore. 2004.
2. H.H. Willard, L.L. Merritt, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, 7th ed., CBS Pub. New Delhi Reprint, 2004.
3. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd ed., John Wiley, New York, 1976.
4. G. D. Christian, Analytical Chemistry, 5th ed, John Wiley & Sons, New York, 1994.
5. J. H. Kennedy, Principles of Analytical Chemistry, 2nd ed., Saunders Holt, London, 1990.

CH521: NANOMATERIALS

(Credits: 03, Lectures: 45)

Unit I

3L

Introduction: Definitions, historical development of nanomaterials, classification of nanomaterials

Unit II

12L

Fundamentals: Size & scale units scaling atoms, molecules, clusters and supramolecules, structure and bonding in nanomaterials chemical bonds (types and strength) intermolecular forces molecular and crystalline structures hierarchical structures bulk to surface transition, surface reconstruction

Unit III

10L

Nanomaterial Synthesis: Chemical routes electrochemical methods vapor growth thin films methods: chemical vapor deposition, physical vapor deposition (sputtering, laser ablation), Sol-gel methods.

Unit IV

10L

Nanomaterial characterization techniques: Scanning and Transmission Electron Microscopy Scanning Probe Microscopies: Atomic Force, scanning tunneling microscopy Diffraction and scattering techniques Vibrational spectroscopy Surface techniques

Unit V

10L

Applications: Nano-electronics Nano optics Nanoscale chemical- and bio-sensing Biological/bio-medical applications Photovoltaic, fuel cells, batteries and energy-related applications High strength nanocomposites Nanoenergetic materials

Reference Books

1. Frank J. Owens and Charles P. Pooler, The Physics and Chemistry of NanoSolids by Wiley-Interscience, 2008.
2. A.S. Edelstein and R.C. Cammarata, Nanomaterials- Synthesis, Properties and Applications, Edited , Institute of Physics Publishing, London, 1998
3. G. Ozin and A. Arsenault, Nanochemistry: A Chemical Approach to Nanomaterials, RSC Publishing, 2005.
4. Edward L. Wolf, Nanophysics and Nanotechnology: An Introduction to Modern Concepts in Nanoscience, Wiley-VCH, 2nd Reprint (2005)

Discipline Specific Electives (DSE-IV) (Select any one)

CH523: BIOMOLECULES-II

(Credits: 03, Lectures: 45)

UNIT-I

10L

Enzymes: Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

UNIT-II

10L

Vitamins: introduction and classification, structure and synthesis, and, biochemical functions and hypervitaminosis of following vitamins: Vitamin A, Vitamin D, Vitamin K, Vitamin C, Vitamin B₁, Vitamin B₂, Vitamin B₆, Vitamin B₇ (Biotin), Vitamin B₁₂, Niacin, pantothenic acid, Folic acid, interrelation between Folic acid and Vitamin B₁₂, vitamin like compounds (choline, inositol, lipoic acid, PABA, bioflavonoids)

UNIT-III

08L

Alkaloids: Introduction, occurrence, nomenclature, classification, physiological action and isolation of alkaloids, Determination of molecular structure of alkaloids: general method, Alkaloids of pharmaceutical importance: Ephedrine, Nicotine, Quinine, Morphine and piperine

UNIT-IV

10L

Terpenoids: Introduction, occurrence, classification, characteristics, Isoprene Rule, general methods for determination of structure of Terpenoids, Hemiterpenoids, Terpenes, Structure elucidation and synthesis of the following terpenoids

Acyclic Monoterpenoids- Geraniol, cyclization reaction of acyclic monoterpenoids

Monocyclic Monoterpenoids – α -Terpineol,

Bicyclic Monoterpenoids- α -Pinene, Camphor

UNIT-V

07L

Carotenoids: Introduction, classification, characteristics, isolation and separation of carotenoids, Principal methods in elucidating the constitution of carotenoids

Structure elucidation and synthesis of the following Carotenoids: α -Carotene, β -Carotene, γ -Carotene, Lycopene.

Reference Books:

1. Organic Chemistry, Vol 2, I. L. Finar, ELBS,2002.
2. K Anand Solomon, Chemistry of Natural Products, MJP Publishers,2012
3. Bhimsen A. Nagasampagi, Meenakshi Sivakumar, and Sujata V. Bhat, Chemistry of Natural Products, Springer,2005.
4. Alagarsamy, Pharmaceutical Chemistry of Natural Products, 2012
5. Text book of Medicinal Chemistry by Madhu Chopra V. K. Ahluwalia, Publisher; Ane Books Pvt. Ltd.2010

CH 525: SOME INDUSTRIAL CHEMICALS

(Credits: 03, Lectures: 45)

UNIT- I

11L

Dyes Industries: Introduction, Classification of Dyes, Colour and Contribution – Valence Bond Theory, M. O. Theory, Witt’s Theory, Synthesis of Fast Red A, Naphthol Blue Black 6B, Naphthol Green B, Rosaniline, Alizarin pyronene

UNIT-II

12L

Oils and Oleochemicals Industries: Introduction, Properties and classification of oils, extraction and purification of oils; Fatty acids Introduction, nomenclature and applications of fatty acids; Soap- Introduction, classification, uses and manufacturing process of soap(s), Manufacture of detergents.

UNIT-III

12L

Cosmetics Industries: Introduction, manufacturing process of powder, cream and lotion, lipstick and nail polish, shampoo and hair dyes, tooth paste.

Perfumery Industries: [Compounds used for different perfumes, Essential oils, Preparation of phenyl ethanol, Yara-Yara, β ionone, musk ketone, musk ambrette, musk xylene, phenyl acetic acid and its’ esters, benzyl acetate, synthetic musk, jasmine.

UNIT-IV

10L

Petrochemicals: Petroleum refining, outline of chemicals derived from ethylene, xylene and naphthalene.

Biofuels: Introduction, Types of biofuels (bioethanol, biodiesel), Raw materials for synthesis of biofuels, Properties of biofuels, biofuels and environment, biofuels and economic, standard specification of biofuels uses of biofuels, Modification of vegetables of oils as biodiesel.

References Books:

1. George T. Austin ,Chemical Process Industries – Shrieves,5thed., McGraw Hill Education, 2017
2. G.R. Chatwal, Synthetic Dyes, Himalya Publishing House, 200
3. Martini, Norbert, Schell, Jozef S., Plants Oils as fuels: Present Science and Future Developments, Springer, 2009
4. Iwata, Hiroshi, Shimada, Kunio Formulas, Ingredients and Production of Cosmetics, Springer, 2013.
5. Billot and F. V. Wells, Perfumery Technology- B. Billot and F. V. Wells, Longman Higher Education; 2nd edition (May 27, 1981)
6. Ashish Thapliyal, Girijesh Kumar Patel, and Vikash Babu, Biofuel Production, Willy, 2013

CH 507: LABORATORY- V

(Credits: 04, Lectures: 60)

1. **Biomolecules:** Isolation, identification and UV determination of, Isolation of following Biomolecules
 - i. Nicotine from tobacco
 - ii. Eugenol from Cloves
 - iii. Curcumin from turmeric
 - iv. Strychnine from Nux Vomica
 - v. Piperine from Black Pepper
2. **Synthesis/Isolation and Evaluation of Antimicrobial activity of following drugs**
 - i. Antitubercular agent: Synthesis of p-aminosalicylic acid from benzene
 - ii. Antibacterial: Synthesis of Sulphanilamide from p-chlorobenzene
 - iii. Antipyretic: Synthesis of Phenacetin from phenol
 - iv. Anti-inflammatory: Salicin from salicylaldehyde
 - v. Cardiovascular agents; Isolation and Identification of reserpine from Rauwolfia serpentine.
3. **Chemicals in Industry**
 - i. Preparation of dyes (any three) Sudan- I, Yellow chrome, orange chrome, Prussian blue
 - ii. Determination of iodine, acid and Saponification values in oils
 - iii. Evaluation of CMC of surfactant solution using surface tension method.

- iv. Preparation of talcum powder.
- iv. Preparation of shampoo.
- v. Preparation of hair remover.
- vi. Preparation of face cream.
- vii. Preparation of nail polish and nail polish remover.

Reference Books:

1. E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK 1990.
2. P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
3. Mark Anthony Benvenuto. *Industrial Chemistry: For Advanced Students*, Walter de Gruyter GmbH & Co KG, 2015
4. Anees A. Siddiqui), *Natural Products Chemistry Practical Manual for Science and Pharmacy Courses 1st*, CBS 2008 .
5. H.T. Clarke and revised by B.Maynes, *2.A Handbook of Organic Analysis Qualitative and Quantitative*, Edward Arnold (Pub.), Ltd. London, 1975.
6. Systema H.Middleton, *tic Qualitative Organic Analysis"* H.Middleton, Edward Arnold (Publishers) Ltd., London 1959.
7. Arthur I. Vogel *A Text Book of Practical Organic Chemistry including Qualitative Organic Analysis"* by, Longmans Green and Co., Ltd., London 2002.
8. William Kamp, *Organic Spectroscopy'*, 3rd ed.. John Wiley & Sons. 2008

CH 509: LABORATORY- VI

(Credits: 04, Lectures: 60)

1. Nanomaterials

- i. Estimation of Carbohydrate by Spectrophotometric method Synthesis of ZnO nanoparticles by sol-gel method.
- ii. Microwave assisted synthesis of ZnO nanoparticles
- iii. Synthesis of ZnO nanoparticles by sonication route

2. Catalysis

- i. To compare the performance of homogenous and heterogeneous catalyst by condensation reaction.
- ii. To compare the performance of heterogeneous catalyst via conventional and microwave method in condensation reaction.
- iii. To check the catalytic activity of photocatalyst in degradation of dyes.

3. Polymers

- i. Synthesis of a polymer (Polystyrene)

- ii. Preparation of poly (vinyl acetate) from PVA
- iii. Determination of epoxy equivalent of a polymer
- iv. Determination of saponification value of a polymer
- v. Determination of acid value of a polymer
- vi. Determination of hydroxyl value of a polymer
- vii. Determination of iodine value of a polymer

4. Organic syntheses using aqueous medium and microwave energy

Reference Books:

1. Experiments in Polymer Science, D. G. Hundiwale, V. D. Athawale, U. R. Kapadi, V. V. Gite, New Age International Pvt. Ltd., New Delhi, 2009.
2. Polymer Chemistry-Practical Approach in Chemistry, F. J. Davis, Oxford University Press, Oxford, 2004.
3. B. Viswanathan, S. Kannan, R.C. Deka, Catalysts and Surfaces: Characterization Techniques, Narosa, New Delhi, 2010
4. G. Ozin and A. Arsenault, Nanochemistry: A Chemical Approach to Nanomaterials, RSC Publishing, 2005