M.Sc. Chemistry

Syllabus

(with effect from 2021)

DEPARTMENT OF CHEMISTRY

The Gandhigram Rural Institute – Deemed to be University

Gandhigram – 624 302 TamilNadu

TEMPLATE FOR PG PROGRAMME

S.NO	CATEGORY	NO. OF CREDITS
1.	Gandhi in Everyday Life	02
2.	Communication and Soft skills	02
3.	Village Placement Programme	02
4.	Human Value and Professional Ethics	02
		08
S.	Core Courses i)Dissertation ii) Modular Course: (2 Courses) iii) Electives: a) Discipline Centric (1course) b) Generic (1 course) iv)Major Course : Minimum 60credits Maximum 72 credits (Theory and Practical) iv)Internship/Field visit (if required)	06 04 03 03 60- 72
		16
	Total	84-96

Semester-wise credits distribution for M. Sc. Chemistry-2021

Template for PG Programme

Course code	Title of the Course	Credits	Hours		Max Marks		
			Theory	Practical	CFA	ESE	Total
FIRST SEMESTER							
21CHEP0101	Inorganic Chemistry -I	4	4	-	40	60	100
21CHEP0102	Organic Chemistry – I	4	4	-	40	60	100
21CHEP0103	Physical Chemistry – I	4	4	-	40	60	100
21CHEP0104	Analytical Chemistry	4	4	-	40	60	100
21CHEP0105	Organic Chemistry Practical-I	2	-	5	60	40	100
21CHEP0106	Physical Chemistry Practical–I	2	-	5	60	40	100
21GTPP0001	Gandhi in Everyday Life	2	2	-	50	-	50#
Total		**22**	**18**	**10**			
SECOND SEMESTER							
21CHEP0207	Inorganic Chemistry – II	4	4	-	40	60	100
21CHEP0208	Organic Chemistry – II	4	4	-	40	60	100
21CHEP0209	Physical Chemistry – II	4	4	-	40	60	100
21CHEP0210	Inorganic Chemistry Practical-I	2	-	5	60	40	100
21CHEP0211	Physical Chemistry Practical– II	2	-	5	60	40	100
21CHEP02GX	Generic Elective	3	3	-	40	60	100
21CHEP2VSX	Value Added Course	2	2	-			
21ENGP00C1	Communication and Soft Skills	2	2	-	50	-	50#
Total		**23**	**19**	**10**			

*** Course code will be given by the respective department offering the course**

 # Not included for CGPA calculation

THIRD SEMESTER							
21CHEP0312	Inorganic Chemistry -III	3	3	-	40	60	100
21CHEP0313	Organic Chemistry – III	3	3	-	40	60	100
21CHEP0314	Physical Chemistry – III	3	3	-	40	60	100
21CHEP0315	Inorganic Chemistry Practical-II	2	-	5	60	40	100
21CHEP0316	Organic Chemistry Practical-II	2	-	5	60	40	100
21CHEP0317	Mini-Project	1	-	-	50	-	50
21CHEP03DX	Discipline Centric Elective	3	3	-	40	60	100
21CHEP03MX	Modular Course	2	2	-	50	-	50
21EXNP03V1	VPP	2	-	-	50	-	50[#]
Total		**21**	**14**	**10**			
FOURTH SEMESTER							
21CHEP0418	Inorganic Chemistry –IV	4	4	-	40	60	100
21CHEP0419	Organic Chemistry – IV	4	4	-	40	60	100
21CHEP0420	Physical Chemistry – IV	4	4	-	40	60	100
21CHEP04MX	Modular Course	2	2	-	50	-	50
21CHEP0421	Dissertation	6	-	12	75	75+ 50	200
21CHEP4VS4	Human Values and Professional Ethics	2	2	-	-	--	-
Total		**22**	**16**	**12**			
Grand Total		**88**	**67**	**42**			

*** Course code will be given by the respective department offering the course**

[#] **Not included for CGPA calculation**

LIST OF DISCIPLINE CENTRIC ELECTIVE COURSES OFFERED (4 credits)

1. 21CHEP03E1 - Polymer Chemistry
2. 21CHEP03E2 - Physical Organic Chemistry
3. 21CHEP03E3 - Medicinal Chemistry
4. 21CHEP03E4 - Environmental Chemistry
5. 21CHEP03E5 - Supramolecular Chemistry
6. 21CHEP03E6 - Advanced Methods in Organic synthesis
7. 21CHEP04M3 - Green Methods in Chemistry

LIST OF GENERIC ELECTIVE COURSES OFFERED (4 credits)

1. 21CHEP02G1 - Elements of Biochemistry
2. 21CHEP02G2 - Instrumental Methods of Chemical Analysis
3. 21CHEP02G3 - Pollution and its Control Measures

LIST OF MODULAR COURSES OFFERED (2 credits)

1. 21CHEP03M1 - Advanced Functional Materials
2. 21CHEP03M2 - Nanotechnology and its Applications
3. 21CHEP04M1 - Molecular Electronics and Organic Photovoltaics
4. 21CHEP04M2 - Water Quality Monitoring, Management and Treatment

LIST OF VALUE ADDED COURSES OFFERED (2 credits)

1. 21CHEP02VA1 - Design thinking innovation and product development
2. 21CHEP02VA2 - Computation tools in chemistry
3. 21CHEP02VA3 - Materials for biological applications
4. 21CHEP04VA4 - Human Values and Professional Ethics

M.Sc. CHEMISTRY (I SEMESTER)

21CHEP0101 INORGANIC CHEMISTRY–I (4 credits)

Objectives: The objective of the course is to develop an understanding of both structure and chemical bonding of inorganic compounds and the basic concepts of acids and bases.

Course outcome: At the end of the course, students will be able to:

- *Predict the chemistry and theories involved in the structure of ionic compounds.*
- *Assess the types of hybridization involved in ionic solids.*
- *Identify the type of crystal structure exist in ionic solids.*
- *Describe the type of defects in metals, band theory and solid state reaction.*
- *Appreciate the basic concepts of acid-bases and theories involved init.*

Unit I - Bonding Models I

Ionic bond - Lattice energy and determination - Born-Lande equation with derivation - Importance of Born Mayer equation and Kapustinskii equation - Application of Born-Haber type calculations - Size effects - Ionic radii - Factors affecting ionic radii - Lewis structure - VB theory. Molecular orbital theory - Symmetry and overlap - Molecular orbitals diagram of diatomic and triatomic molecules - Formal charge.

Unit II - Bonding Models II

Hybridization - Molecular orbital equivalent of hybridization-Delocalization - Resonance - Molecular orbital equivalent of resonance. Fajan's rule - Results of polarization - Covalent bonding in ionic solids - polarizing power - polarizability- Charge distribution in molecules - Dipole moment - Determination and applications.

Unit III – Solid State Chemistry I

Cells and description of crystal structure-symmetry-seven crystal systems - Close packing of spheres - Packing efficiency - Hexagonal close packed (HCP) and cubic close packed structures (CCP) - Coordination number - Relative density of packing in simple cubic, CCP, HCP and BCC - Tetrahedral and octahedral holes - Limiting radius ratio rule.

Radius ratio for trigonal, tetrahedral, octahedral and cubic sites - Radius ratio and shape of ionic crystals - Structures of cesium chloride, sodium chloride, zinc blende, fluorite, rutile andcalcite.

Unit IV – Solid State Chemistry II

Perovskite structure of spinels - Stoichiometric defects - Schottky and Frenkel defects - Non-stoichiometric defects - Metal excess and metal deficiency defects - Extended defects - Line and plane defects. Band theory - Semiconductors - Intrinsic and extrinsic type - Fermi level- Flow of current in semiconductors - Hopping mechanism - Band structure - p and n type

semiconductors - p-n junction - Superconductivity - 1,2,3-superconductor – Photovoltaic effect. Solid state reactions - Classification - Thermal decomposition reactions - Reaction between two solids - Improving reactivity ofsolids.

Unit V - Acid-Base Concept

Acid-Base concept- Solvent system concept - Bronsted Lowry- Lux-Flood - Lewis concept and Usanovich concept - Classification of Lewis acids - Lewis acid-base reactions - nonaqueous solvent and acid base strength- super acids - Solvolysis and formation of coordination compounds.

Hard and Soft Acids and Bases (HSAB) – Theory of Hard and Soft Acids and Bases – Applications of HSAB theory - - Strength of oxyacids - Pauling's rule - Acidity of cations in aqueous solution- solvation and acid base strength- Factors affecting relative strength acids and bases-substituents-steric effect-resonance effect.

References:

1. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and CH.Langford, ELBS, Oxford University Press, 6thEdn.,2015.
2. Inorganic Chemistry, J.E. Huheey, E.A. Keither and R.L. Keiter, Harper Collins College Publisher, New York, 4th Edn.,1993.
3. Modern Inorganic Chemistry, W.E. Jolly, McGraw Hill International Edition, New York,1994.
4. Theoretical Principles of Inorganic Chemistry, G. S. Manku, Tata McGraw Hill Publishing Company Ltd., New Delhi,1994.
5. Concepts and Models of Inorganic Chemistry, B.Douglas, D.H.Me Daniel and J.J. Alexander, John Wiley and Sons, New Delhi,2001.
6. Solid State Chemistry, D.K. Chakrabarthy, New Age International Publishers, NewDelhi, 2005.

21CHEP0102 ORGANIC CHEMISTRY - I (4 credits)

Objectives: The objective of the course is to develop an understanding of reactivity organic compounds, reaction mechanisms and synthetic utility of some important organic reagents and characterization of organic compounds by NMR. The course also will give an understanding of the chemistry of some selected heterocyclic compounds.

Course outcome: At the end of the course, students will be able to:

- *Assess the thermodynamic and kinetic controlled products and methods of determination of reaction mechanisms.*
- *Describe and formulate the mechanism of various nucleophilic substitution reactions and elimination reactions.*
- *Elucidate the structure of organic compounds using NMR spectroscopy.*
- *Assess the mechanism and synthetic uses of selected reagents.*
- *Describe the chemistry of Nitrogen and oxygen heterocycles*.

Unit I – Methods of Determination of Reaction Mechanisms and Aromaticity

Thermodynamic and Kinetic Requirements of Reactions: Thermodynamic and kinetic control – methods of determination of reaction mechanisms – product analysis – determination of the presence of intermediate, isolation, detection, trapping – cross over experiments – isotopic labeling – isotopic effect – stereo chemical evidence – kinetic evidence.Kinetic Methods of Determination of Reaction Mechanisms: Hammett equation – significance of substitution and reaction constant – Hammond postulates – Linear free energy relationship – limitations and deviations – Taft equation.

Aromaticity: Conditions for aromaticity, Aromatic systems with 2,6,10 electrons, alternent and non-alternent hydrocarbons, systems of more than 10 electrons annulenes-aromaticity of azulenes, ferrocene and sydnones - Aromatic, nonaromatic, antiaromatic systems- concept of homoaromaticity.

Unit II – Reaction Mechanism

Reaction Mechanism: Nucleophilic substitution at saturated carbon atom- S_N1 and S_N2 reactions- mechanism and evidences- effect of structure- solvent- stereochemistry- S_Ni, S_N1', S_N2', S_N1cA and S_N2cA mechanism-Neighbouring group participation- Non classical carbocations. S_NAr mechanisms. Elimination Reactions: E1, E2 and E1cB – evidences – effect of structure, solvent and base – Hoffmann and Saytzeff rules – stereochemistry of E1 reaction – Pyrolytic elimination – cis elimination – elimination vs substitution.

Unit III - Organic Reagents-I

Study of synthetic applications of the following reagents - LDA, LiHMDS, ^{n}BuLi – ortholithiation, DMAP, DDQ, $Pd(PPh_3)_4$, Simmon-Smith Reagent, Gilman's Reagent, Woodword & Prevost Hydroxylation and Peterson's Synthesis.

Unit IV – Chemistry of Heterocyclics

Oxygen Heterocyclics: Classification, color reactions of various classes of flavonoids – chemistry and synthesis of flavones (luteolin), isoflavones (daidzein), flavonols (kaempferol) and anthocyanidins (cyanidin).

Nitrogen Heterocyclics: Synthesis and reactivity of indole, pyrazole, imidazole, pyrimidines – uracil, cytosine, purines – adenine, guanine and caffeine.

Unit V – NMR Spectroscopy

NMR Spectroscopy: ^{1}H–NMR spectroscopy: Chemical shifts – spin-spin coupling – coupling constant – analysis of first order spectra – spin-spin splitting – shielding, deshielding, anisotropic effect – AX, AX_3, A_2X_3, AMX, ABX, AB_2, A_2B_2 systems – Karplus equation – factors influencing the coupling constant J – influence of stereochemical factors on chemical shift of protons – Protons-deuterium exchange phenomenon, chemical spin decoupling of rapidly exchangeable protons (-OH, -SH, -COOH, -NH, $-NH_2$) – non I order spectra – simplification of complex spectra – double resonance – shift reagents – NOE and its applications.

^{13}C-NMR spectroscopy: low natural abundance – ^{1}H decoupling – off resonance study – effect of alkyl and halogen substitution, hybridization effects. Basic principles of 2D NMR spectroscopy – NOESY, COSY.

References:

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.
2. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st edition, Oxford University Press, 2001.
4. G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006.
5. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4th edition Cambridge University Press.
6. H. O. House, Modern Synthetic Reactions, Benjamin-Cummings Publishing Co. 2nd edition, 1972.
7. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spectrometric identification of organic compounds, 7th edition, John Wiley, 2005.

8. Organic Spectroscopy, W. Kemp, 3rd edition, Macmillan, 2011.
9. D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, McGraw Hill, 6th edition 2007.
10. D. L. Pavia and G. M. Lampman Spectroscopy 4th Edition, Brooks Cole, 2012. 5. H. Gunther, NMR Spectroscopy Wiley-VCH, 2013.
11. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2007.
12. I.L. Finar, Organic Chemistry, Vol.2 ELBS, 5th edition, 1974 and Pearson India, 5th edition, 2011.

21CHEP0103 PHYSICAL CHEMISTRY–I (4credits)

Objectives: The content of this course is designed to give the knowledge of different laws of thermodynamics and various concepts of electrochemistry. The course also emphasizes the importance of rechargeable batteries and fuel cells.

Course outcome: At the end of the course, students will be able to:

- *Assess the basic concepts in reversible and irreversible thermodynamics.*
- *Describe the basic theories at the electrolyte-electrode interfaces.*
- *Outline the electrochemical principles involved in corrosion and energy storage devices.*
- *Identify the different types of fuel cells and discuss their merits and demerits.*

Unit I - Thermodynamics and Non-ideal Systems

Chemical potential, Gibbs-Dhhem equation, variation of chemical potential with temperature and pressure. Fugacity-definition. Determination of fugacity of gases by graphical method and from equations of state. Variation of fugacity with temperature and pressure. Fugacity and the standard state for non-ideal gases. Fugacity and mixtures of non-ideal gases, chemical equilibrium involving non-ideal gases. Physical significance of fugacity. Definition of activity and activity coefficient-variation of activity with pressure and temperature-determination of activity and activity coefficient of non-electrolytes. Lewis Randal rule-Duhem-Margules equation.

Unit II -Third Law of Thermodynamics and Chemical Equilibrium

Third law of thermodynamics, Nernst heat theorem, unattainability of absolute zero, calculation of absolute entropies based on third law of thermodynamics, residual entropy and its application. Virial equation of state.

Chemical equilibrium-Thermodynamic derivation of equilibrium constant for equilibrium involving ideal and real gases-Temperature dependence of the equilibrium constant-Vant-Hoff equation.

Unit III - Non-equilibrium Thermodynamics and Phase Rule

Basic concept of non-equilibrium thermodynamics-postulates and methodologies-linear laws-Entropy of irreversible processes-Clausius in equality-entropy production (heat flow, chemical reactions, electrochemical reactions) and entropy production in open systems-phenomenological equations-Onsager reciprocity relation.

Phase equilibrium: Gibbs phase rule-derivation-applications to three component systems-Graphical representation-Systems of three liquids-systems consisting of two salts and water.

Unit IV-Electrochemistry I

Electrical double layer: Structure of electrical interface, parallel plate condenser model, Gouy-Chapmann diffused charge model, Stern model, limitations of these models. Semiconductor interfaces, Theory of double layer at semiconductor-electrolyte solution interfaces, Lippman equation. Electrocatalysis-influence of various parameters. Butler-Volmer equation-low field and high field approximations-Tafel equation. Thermodynamics and kinetics of electrochemical metal deposition and dissolution process (corrosion), mechanism, corrosion current, Evan's diagram, Protection and prevention of corrosion.

Unit V- Electrochemistry II

Ionic strength-Debye Huckel theory-Debye-Huckel limiting law-relaxation effect-electrophoretic effect-Debye-Huckel-Onsager (DHO) conductance equation - validity of DHO equation-deviations from the DHO equation. Conductivity at high frequency and at high field strength. Debye – Falkenhagen effect and Wien effect

Lead-acid batteries-Cadmium-Nickel oxide batteries-charging and discharging reactions-Lithium rechargeable batteries. Fuel cells-classification-chemistry of fuel cells- detailed description. Supercapacitors-types of supercapacitors.

References:

1. Electrochemical Methods Fundamentals and Applications, Allen J. Bard and Larry R. Faulkner 2nd Edn., John Wiley and Sons,2004.
2. Fuel Cells-Principles and Applications, B.Viswanathan, M.Aulice Scibioh, Universities Press, Hyderabad, India,2006.
3. Modern Electrochemistry, John M. Bockris and Amulya K.N. Reddy, Vol. I & II, 2nd Edn., Springer, New Delhi,2000.
4. Physical Chemistry, P.W. Atkins, Oxford University Press,1998.
5. Thermodynamics for students of Chemistry, Kuriakose and Rajaram, Shoban Lal Nagin Chand,1986.D.R. Crow, Principles and Applications

21CHEP0104 ANALYTICAL CHEMISTRY–I (3 credits)

Objectives: The objective of the course is to give the students an in-depth account of various modern analytical techniques like spectrophotometry, XRD, radiometry, thermal and electroanalytical techniques with a view to understand the principles, instrumentation and applications. The course also gives account of statistical treatment of data and chromatographic techniques.

Course outcome: At the end of the course, students will be able to:

- *Analyze the accuracy and precision of the statistical data.*
- *Summarize the principles and applications of AAS and XRD.*
- *Describe the different thermal methods and radiometric titrations.*
- *Apply different electroanalytical techniques for the detection of metal ions at trace level.*

Unit I - Statistical Treatment of Data, Separation Techniques and Intellectual Property Rights

Errors-classification-minimization of errors-accuracy, precision, standard deviation, coefficient of variance, Q-test and t-test, significant figures, rules for rejection of analytical data.

Chromatography-principles, instrumentation and applications of GC and HPLC, Ion-exchange techniques.

Solvent extraction - factors favoring solventextraction-Batch and Continuous process.

Introduction to Intellectual Property: Historical Perspective, Different Types of IP, Importance of protecting IP. Patent: Introduction, patenting process and requirements of patenting.

Unit II - Spectrophotometry and XRD

Atomic absorption spectrophotometry (AAS)-principle, instrumentation and applications, types of interferences. Flame emission spectroscopy (FES)-theory, instrumentation and applications-Difference between AAS and FES.

Inductively coupled plasma atomic emission spectroscopy (ICEP-AES) and inductively coupled plasma mass spectrometry (ICP-MS)-principle and applications.

XRD-principle- single crystal-powder crystal methods andapplication.

Unit III - Radiochemical and Thermal Methods of Analysis

Isotopic dilution methods-direct and inverse-neutron activation analysis. Absolute and comparator methods-Radiometric titrations-types – applications.

Principles, instrumentations and applications of thermogravimetry, Differential thermal analysis and differential scanning calorimetry-thermograms of calcium oxalate monohydrate and copper sulphate pentahydrate.

Unit IV - Electroanalytical Techniques I

Polarography-principle-polarographic maxima-Ilkovicequation-Half-wave potential-applications. Cyclic voltammetry-principle-interpretation of cyclic voltammogram for a reversible couple- -simple analytical applications-chemically modified electrodes-modification of electrodes by different methods-ultramicroelectrodes in voltammetry-Differential pulse voltammetry.

Unit V - Electroanalytical Techniques II

Basic principles of coulometry-coulometry at controlled potential-coulometry at constant current-coulometric titrations-advantages and applications-theory of chronopotentiometry and chronoamperometry. Anodic stripping voltammetry-principle and applications-ion selective electrodes-characteristics-different types-principle and applications.

References:

1. Instrumental methods of analysis, H,W. Willard, L.I. Merrit, J.J.A. Dean and F.A. Settle, CBS publishers,1983.
2. Principles of Instrumental methods of analysis, Skoog and West, Saunders College Publications, 1992.
3. Instrumental methods of chemical analysis, B.K. Sharma, Goel publishing House, 19th Edn.,2000.
4. Electrochemical Methods, Fundamentals and Applications, A.J. Bard and L.R. Faulkner, John Wiley & Sons, 2nd Edn.,2001.
5. Intellectual property rights in the WTO and developing countries, J.Watal,Oxford University Press, Oxford,2001.
6. Principles of Instrumental methods of analysis, D. A. Skoog, F. J. Holler, F. J. and R. Stanley, Boston: Cenage Learning, 7thEdn, 1992.

M.Sc. CHEMISTRY (I SEMESTER)

21CHEP0105 ORGANIC CHEMISTRY PRACTICAL–I (2 credits)

Objectives: The practical course is designed to acquire skill in separation and qualitative analysis.

Course outcome: At the end of the practical course, students will be able to:

- *Adopt different laboratory techniques for crystallization and sublimation.*
- *Formulate strategies for the separation and qualitative analysis of two and three component mixtures of organic compounds.*
- *Plan for the preparation of desired organic compounds, extraction and purification of organic compounds*

1. Different laboratory techniques-Melting point, Distillation-at atmospheric pressure-at reduced pressure, TLC, Column Chromatography, Crystallization, Sublimation, Preparation of dry solvents.
2. Separation and qualitative analysis of two component mixtures of organic compounds-Characterization of derivatives and identification of the components.
3. Single stage preparation of organic compounds using classical organic reactions such as nitration, bromination, acetylation, condensation and oxidation by green approach.
4. Extraction of caffeine from tea leaves, piperine from pepper, lachanoric acid from lichens and casein from milk.

References:

1. Vogel's Text Book of Practical Organic Chemistry, Furniss, S. B.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. 5Th Ed.; Longman Scientific & technical, England, 1989.
2. Laboratory Manual of Organic Chemistry, Dey and Sitaraman, Allied Publishers, 1992.

21CHEP0106 PHYSICAL CHEMISTRY PRACTICAL–I (2credits)

Objectives: The practical course is designed to set-up different electrochemical cells and to carry out different applications of potentiometric, pH metric, conductometric titrations and to verify the theories by conductometry method.

Course outcome: At the end of the practical course, students will be able to:

- *Set-up of different electrochemical cells Analyze the dissociation constant and solubility product by conductometry and potentiometry respectively.*
- *Identify the thermodynamics of simple systems.*
- *Assess and adopt the conductometric methods to verify the theories*

1. Setting up of various cells and measurement of their values, Examples: Zn /0.1M $ZnSO_4$/ KCl / Hg_2Cl_2 / Hg / Ag / AgCI / 0.l M KCl / Hg_2Cl_2/ Hg/ Hg_2Cl_2/ KCl/ 0.1 M $CuSO_4$/Cu.
2. Determination of redox potentials and equivalence points from potentiometric titration.
3. Determination of the solubility and solubility product of silver chloride in water potentiometrically.
4. Potentiometric titration of a mixed solution of KCl and KI against$AgNO_3$.
5. Determination of dissociation constant of a weak acid by pH metric titration.
6. pH metric titration of mixture of weak acid and strong acid against strong base.
7. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
8. Experimental verification of Debye-Huckel-Onsager equation.
9. Conductometric titration of a mixture or a weak acid and strong acid against a strong base.
10. Determination of neutralization enthalpy of HCl and CH_3COOH by NaOH.
11. Determination of solution enthalpy by thermometric method. Oxalic acid-water, $K_2Cr_2O_7$-water and naphthalene -toluene.

References:

1. Experimental Physical Chemistry, G. Peter Mathews, Oxford Science Publications, 1985.
2. Experimental Physical Chemistry Ed, by E. Danielset al., International student edition, McGraw Hill KogakushaLtd.,1970.
3. Senior Practical Physical Chemistry, D. D. Khosala, A. Khosala, V. C. Gard, R. Chand & Co., New Delhi,1975.
4. Practical Physical Chemistry, B. Viswanathan and P. S. Raghavan, Viva Books Pvt. Ltd., New Delhi, 2008.

M.Sc. CHEMISTRY (II SEMESTER)

21CHEP0207 Inorganic Chemistry– II (4 credits)

Objectives: The objective of the course is to impart knowledge in bonding,reaction mechanisms and electronic spectra of coordination compounds.

Course outcome: At the end of the course, students will be able to:

- *Explain crystal field theory, crystal field splitting in complexes ,its limitations, and constructing MO diagrams of complexes.*
- *Categorize the mechanical aspects of inorganic complexes.*
- *Describe trans effect, theories of trans effect and redox reactions.*
- *Analyze and interpret the electronic spectra of coordination complexes*.

Unit I - Coordination Chemistry (Bonding)

Crystal field theory (CFT) –Postulates of CFT - Crystal field splitting in octahedral, tetrahedral and square planar complexes - Crystal field stabilization energy and its applications in stereochemistry, stability of oxidation states, trends in heats of hydration & lattice energy and colour& magnetic properties- Weak and strong fields - Pairing energy - Factors affecting the magnitude of crystal field splitting-Jahn-Teller theorem – Limitations of CFT.

Unit II - Coordination Chemistry (Bonding & Properties)

Molecular orbital (MO) theory for octahedral, tetrahedral and square planar complexes **–** Types of pi-bonds-Effect of pi-bonding on crystal field splitting – Experimental evidences for pi -bonding. Symbiosis - Chelate effect – Magnetic properties – Dia, para, ferro and antiferro magnetisms - Curie's law – Spin isomerism. Stability constants of complexes and their determination methods (Ion exchange, electrochemical, polarographic, spectrophotometric and method of continuous variation methods)-Factors influencing stabilityconstants of metal complexes with respect to the nature of metal ion and ligand.

Unit III - Coordination Chemistry (Reaction Mechanism I)

Substitution reactions: General mechanism - Schemes of octahedral, tetrahedral and square planar complexes – Dissociative (D) – Associative (A) - Interchange (I) and dissociation types - Linear free energy relationships- Acid and base hydrolysis reactions-Substitution reaction without M-L bond breaking. Racemisation and isomerisation: Twist mechanisms for isomerisation – Intra molecular mechanisms forracemisation.

Unit IV - Coordination Chemistry (Reaction Mechanism II)

Labile and inert complexes-VBT and CFT-Trans-effect - Theories of trans-effect, pi-bonding theory and polarization theory- Application of trans effect-cis effect. Redox reactions: complementary and non-complementary reactions-Inner sphere mechanism - The role of bridging ligand - Outer sphere mechanism - The limiting rate law - Theoretical treatment of electron transfer - Simple applications to bio-inorganic chemistry.

Unit V - Coordination Chemistry (Electronic spectra of complexes)

Quantum numbers of multi -electron atoms - Russell-Sanders coupling - L-S coupling and micro states – Ground state terms for d^1 – d^{10} ions-Derivation of terms for p^2 , p^3, d^1 and d^2 configurations - Hund's rules in the determination of lowest energy states - Selection rules for electronic transitions – Charge transfer transitions - Ligand to metal charge transfer and metal to ligand charge transfer. Splitting of free ion terms in octahedral field - correlation diagram - Orgel diagrams for $[M(H_2O)_6]^{n+}$ (M = d^1 to d^9 ions) d^1 to d^9 ions and Tanabe-Sugano diagrams for d^2 and d^3 ions.

References:

1. Inorganic Chemistry,J.E.Huheey,E.A.KeitherandR.L.Keiter,HarperCollinsCollegePublisher, 4thEdn., New York,1993.
2. InorganicChemistry,G.L.MiesslerandD.A.Tarr,Pearson,PrenticePublishers,Delhi,2009.
3. InorganicChemistry,D.F.Shriver,P.W.AtkinsandC.H.Langford,ELBS,OxfordUniversity Press,2000.
4. Concepts and Models of Inorganic Chemistry, B. E. Douglas, D.H. McDaniel and J.J. Alexander, John Wiley and Sons, New Delhi,2001.

21CHEP0208 ORGANIC CHEMISTRY – II (4 credits)

Objectives: The objective of the course is to understand various organic reactions and reagents, to have advanced knowledge in UV-vis and IR spectroscopy, to know the chemistry of organic molecules based on conformational analysis, to understand the chemistry of terpenoids.

Course outcome: At the end of the course, students will be able to:

- *To Know the knowledge of UV-vis and IR NMR spectra*
- *Describe and formulate the mechanism of oxidation, reduction, rearrangements reactions and some selected name reactions.*
- *Predict and analyze the conformations of acyclic and cyclic organic compounds.*
- *Elucidate the structure and propose synthesis of selected terpenoids.*

Unit I – UV-vis and IR Spectroscopy

UV-vis spectroscopy: Different regions of electromagnetic spectrum – Electronic energy levels, electronic transitions and selection rules– Factors affecting the position of UV-vis bands – effect of structure and solvents-Woodward- Fischer rules for calculating absorption maxima of conjugated dienes,-α,β-unsaturated carbonyl compounds –Disubstituted benzene derivatives.

IR Spectroscopy: Molecular vibrations- factors influencing vibrational frequencies– group frequency concept- hydrogen bonding- effect of inductive and mesomeric effects on carbonyl stretching frequency- effect of ring strain on carbonyl stretching frequency- applications of IR spectroscopy to organic compounds

Unit II – Organic Reactions (oxidation, reduction and name reactions)

Oxidation: Mechanism and applications of reaction involving oxidation with CrO3, OsO_4, SeO_2, $NaIO_4$, mCPBA and Swern oxidation.

Reduction: Mechanism and applications of reaction involving reduction with $NaBH_4$, $LiAlH_4$, DIBAL-H, Bu_3SnH. Name Reactions: Robinson annulations, Suzuki Coupling, Wittig reaction, Stark enamine synthesis and Shapiro reaction.

Unit III – Molecular Rearrangements

Molecular Rearrangements: 1,2- shifts in carbocations –Curtius, Lossen, Demjanov, Bayer Villiger, Favorski, Benzidine, Nebar, Hoffmann- Loflller- Freytag rearrangement.

Unit IV – Conformational Analysis

Conformational Analysis of acyclic system: conformation of halogenoalkanes, conformation of diastereomers- conformational effects on reactivity- acyclic systems only- addition reactions- elimination reactions.

Conformational Analysis of Cyclic Compounds: cyclohexane- chair, skew boat- boat conformations- mono and disubstituted cyclohexane-stable conformer- physical properties-Von Auwers Skitta rule- conformations of cis and trans decalins. Conformations of perhydroanthracene and perhydrophenanthracene - conformationally rigid and mobile diastereomer, quantitative correlation between conformation and reactivity, Winstein- Eliel equation, Curtin- Hammett principle, Steric assisted and steric hindered reactions.

Unit V – Terpenoids

Terpenoids: Biogenesis- isoprene rules - classification of terpenoids - structure and synthesis of zingiberene, α-cadinene, α-pinene, camphor and abietic acid.

References:

1. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spectrometric identification of organic compounds, 7th edition, John Wiley, 2005.
2. Organic Spectroscopy, W. Kemp, 3rd edition, Macmillan, 2011.
3. D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, McGraw Hill, 6th edition 2007.
4. D. L. Pavia and G. M. Lampman Spectroscopy 4th Edition, Brooks Cole, 2012.
5. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2007.
6. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Part B, Fifth Edition, 2007
7. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st edition, Oxford University Press, 2001.
8. G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006.
9. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4th edition Cambridge University Press.
10. H. O. House, Modern Synthetic Reactions, Benjamin-Cummings Publishing Co. 2nd edition, 1972.
11. A. J. Kirby, Stereoelectronic Effects, Oxford University Press, 1996.
12. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds Wiley Student Edition, 2008.
13. I.L. Finar, Organic Chemistry, Vol.2 ELBS, 5th edition, 1974 and Pearson India, 5th edition, 2011.

21CHEP0209 PHYSICAL CHEMISTRY–II (4 credits)

Objectives: The objective of the course is to have an introductory idea of quantum chemistry and basic concepts of group theory and its applications.

Course outcome: At the end of the course, students will be able to:

- *Describe the basic concepts and applications of quantum chemistry.*
- *Categorize the operators and Eigen functions.*
- *Formulate the approximation methods to construct molecular orbitals.*
- *Identify the point groups of molecules and apply the concepts of group theory to predict the spectroscopic properties*.

Unit I - Quantum Chemistry I

Success of quantum theory and failure of classical mechanics-experimental foundation of quantum mechanics-black body radiation-photoelectric effect. Compton effect and atomic spectra. Formulation of quantum mechanics-the wave nature of sub-atomic particles-wave particle dualism-Heisenberg's uncertainty principle-Schordinger wave equation. Concept of operators-sums and products of operators-commutator-linear and non-linear operators-Hermitian and Hamiltonian operators- Deriving operators for energy and angular momentum from known operators-Eigen values and Eigen functions-postulates of quantum mechanics-physical interpretation of wave function-orthogonality and normalization theorems.

Unit II - Quantum Chemistry II

Applications of wave mechanics-Schrodinger wave equation to free particle-particle in a one dimensional box-particle in a three dimensional cubic and rectangular box-degeneracy.One dimensional harmonic oscillator-classical treatment of simple linear harmonic oscillator and its limitations-quantum mechanical treatment-complete solutions for linear harmonic oscillator-Hermite polynomial and orthogonality-Normalized solution and energy values. Rigid rotator-rigid rotator as a model fora rotating diatomicmolecule-solutions.

Unit II - Quantum Chemistry III

Solving of Schrodinger equation for the H-atom (or H-like species)-energy levels-quantum numbers radial factors and angular parts. Atomic orbitals and their shapes-electron spin and Pauli's exclusion principle.-approximation methods-need for approximation methods-Perturbation theory (I order only)-application to H-like atoms-Variation method-Application to helium atom-Molecular orbital theory- LCAO-MO treatment-MO theory of simple heterodiatomic molecules like HF, LiH, CO andNO.

Unit -IV Basics of Group Theory

Definition of a mathematical group and its properties – symmetry elements - symmetry operations – classes of symmetry operations - group multiplication table - cyclic groups-subgroups - classes –classification of molecular point groups. Matrix representations of symmetry operations-representation of groups-reducible and irreducible representations. The Great Orthogonality theorem and its consequences-character tables – construction of character tables for C_{2v} and C_{3v} pointgroups.

Unit – V Applications of Group Theory in Chemistry

Group theory and quantum mechanics – direct product - wave function as bases for irreducible representation - Symmetry Adapted Linear Combinations (SALC)-projection operators and their use to construct SALC-Huckel approximation-concept of hybridization-hybridization in methane - secular determinant – symmetry factoring of secular equations-□-MOs for butadiene, benzene - spectral transition probabilities -electronic spectra-selection rule-electronic transition in formaldehyde- vibrational spectra – normal modes of vibration - selection rules – mutual exclusion principle-IR and Raman activity of fundamentals in H_2O, N_2F_2 and CH_4.

References:

1. Introductory Quantum Chemistry, A.K. Chandra, Tata McGraw-Hill Publishing Company, 4th edn.,1994.
2. Quantum Chemistry, R.K. Prasad, Wiley Eastern, New Delhi,1992.
3. Introductory Quantum Mechanics, Y.R. Waghmare, Eurasia Publishing House, NewDelhi, 1989.
4. Fundamentals of Quantum Chemistry, Anandaraman, MacMillan, India,2001
5. F.A. Cotton, Chemical Applications of Group Theory, 3rdedn., Wiley-Interscience Publications, 2006.
6. A. Salahuddin Kunju and G.Krishnan group theory and its applicationsin Chemistry, Eatern Economy Edition, 2nd edition, PHI Learning Publishers, 2015.
7. P.K. Bhattacharya, Group Theory and Its Chemical Applications, Himalayan Publishing House, 1986.
8. V. Ramakrishnan and M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1998.

M.Sc. CHEMISTRY (II SEMESTER)

21CHEP0210 INORGANIC CHEMISTRY PRACTICAL–I (2credits)

Objectives: The practical course is designed to develop skills in identification of elements by inorganic qualitative analysis and also preparation of some inorganic complexes.

Course outcome: At the end of the practical course, students will be able to:

- *Analyze most common and less common ions by using semi-micro inorganic qualitative methods.*
- *Formulate suitable methods for the preparation of desired inorganic complexes*

1. **Analysis of mixtures containing two common and two less common cations.**

   Ions of the common metals: Pb, Cu, Mn, Cr, Al, Ni, Co, Ba, Sr, Ca, Mg

   Ions of less common metals: W, Se, Te, Mo, Ce, Th, Zr, Ti, V, U, Li.

2. **Inorganic Preparations**

   a. Hexamminecobalt(III) Chloride
   b. Tatraamminecopper(II) Sulphate
   c. Hexaaminechromium(III)Nitrate
   d. Hexaureachromium(III)Chloride
   e. Tris(ethylendiamine)nickel(II) Chloride
   f. Tris(ethylenediamine)chromium(III)Chloride
   g. Potassiumtris(oxalato)ferrate(III)
   h. Potassiumtris(oxalato)chromate(III)
   i. Potassiumtris(oxalato)cuprate(II)
   j. Potassiumhexathiocyanatochromate(III)
   k. Potassiumtetrathiocyanatodiamminechromate(III)
   l. Hexathiourealead(II)nitrate

Reference:

1. Inorganic Semi-Micro Qualitative Analysis, V.V. Ramanujam, The National Publishing House, Chennai,1990.

21CHEP0211 PHYSICAL CHEMISTRY PRACTICAL–II (2credits)

Objectives: The practical course is designed to study the chemical kinetics of different reactions, the adsorption behavior of compounds on solid surfaces, and to determine the concentration of analytes in a mixture by colorimetry.

Course outcome: At the end of the practical course, students will be able to:

- *Determine the kinetics of the reactions.*
- *Analyze physisorption and chemisorptions mechanisms.*
- *Identify the concentration and composition of liquids by refractometry.*
- *Predict the concentration of two analytes in a mixture.*

1. Determination of the temperature coefficient and energy of activation of hydrolysis of ethylacetate.
2. Determination of the rate constant and order of reaction for the reaction between potassium persulphate and potassium iodide.
3. Study of the kinetics of the reactions between iodine and acetone.
4. To determine the rate constant of iodine clock reaction.
5. To study the adsorption of acetic acid/oxalic acid in activated charcoal and verify the Freundlich and Langmuir adsorption isotherms.
6. To determine the relative viscosities of various liquids using Ostwald viscometer.
7. To determine the molecular weight of a polymer by viscosity method.
8. Estimation of concentration of a mixture by colorimetric method.
9. Construction of a phase diagram for a three-component system (toluene/ chloroform-water-acetic acid)
10. To test the validity of Lambert Beer's law for $KMnO_4$ and $K_2Cr_2O_7$ in H_2SO_4.
11. Determine the composition of the binary mixture containing $KMnO_4$ and $K_2Cr_2O_7$

References:

1. Experimental Physical Chemistry, G. Peter Mathews, Oxford Science Publications,1985.
2. Experimental Physical Chemistry Ed, by E. Daniels, International Student Edn., McGraw Hill,1970.
3. Senior Practical Physical Chemistry, D.D. Khosala, A. Khosala, V.C. Gard, R.Chand & Co., New Delhi, 1975.
4. Practical Physical Chemistry B. Viswanathan and P.S. Raghavan, Viva Books Pvt. Ltd., New Delhi, 2008.

M.Sc. CHEMISTRY (III SEMESTER)

21CHEP0312 Inorganic Chemistry– III (3 credits)

Objectives: The objective of the course is to develop an understanding of the chemistry of metal complexes, metallocenes and various reactions of organometallics, to appreciate the use of organometallic reagents in organic synthesis, to understand the chemistry of chains, rings, cages and clusters of inorganic compounds and to gain knowledge on functions of metal ions, mechanistic aspects of photosynthesis, oxygen transport in biological systems.

Course outcome: At the end of the course, students will be able to:

- *Describe the chemistry of metal complexes and interpret the structure of metal carbonyls using IR spectral data.*
- *Select and integrate the chemistry of metalloenzymes and the mechanical aspects of organometallics.*
- *Appreciate the chemistry of chains, rings, cages and clusters.*
- *Describe and evaluate the functions, mechanism of photosynthesis, enzymes and oxygen transport in biological systems.*

Unit I - Organometallic Chemistry I

18 electron rule - Concept of hapticity - Preparation, structure and bonding in polynuclear carbonyl, nitrosyl and dinitrogen complexes-Applications of IR spectra in the study of structure of metal-carbonyls. Preparation, structure and bonding in metal carbenes, carbynes, alkenes, alkynes and allyl complexes.

Unit II - Organometallic Chemistry II

Metallocenes – classification – Preparation, properties and bonding in ferrocene – MO theory - cycloheptatriene and tropylium complexes. Reactions of organometallics: Mechanism of substitution reactions in carbonyl complexes – Mechanism of oxidative addition and reductive elimination and insertion and elimination reactions – C-H activation.

Unit III - Organometallic Chemistry III

Organometallic reagents in organic synthesis: Synthetic importance of iron pentacabonyl and organo palladium complexes. Homogeneous catalysis: Alkene hydrogenation, hydroformylation, Monsanto acetic acid process, Wacker process - photodehydrogenation catalyst- polymerization by Ziegler-Natta catalyst – Isomerization of alkenes.

Unit IV - Chains, Rings, Cages and Clusters Chains

Isopoly anions and heteropoly anions of V, Cr, Mo and W. Rings: Synthesis and reactions of borazines, S-N ring compounds, phosphazenes, phosphazene polymers - Structures and bonding of phosphazene. Cages: Phosphorus, phosphorus trioxide and pentoxide - Borane carborane and metallocarboranes compounds - Higher boron hydride classification and electron counting. Clusters: Dinuclear, tetranuclear and hexanuclear cluster -Polyatomic zintl anions and cations –Chevralphases.

Unit V - Bioinorganic Chemistry

Metal ions in biology- Mechanism of ion transport across membranes-Sodium and potassium pump, Photosynthesis – PS- I, PS-II, Porphyrins, Metalloenzymes- Carbonicanhydrase, superoxide dismutase, xanthine oxidase, nitrogenaseand Carboxypeptidase, Oxygen transport and storage- Hemoglobin, myoglobin, hemerythrin, and hemocyanin. Metal ion transport and storage: Ferritin, Transferrin, Siderophores and metallothionein.Electron Transfer- Cytochromes, Iron-Sulfur Proteins and Copper Proteins -Nitrogen fixation- anti cancer activity of platinum complexes (cisplatin and carboplatin).

References:

1. Inorganic Chemistry, 4thedn., J.E. Huheey, E.A. Keither and R.L. Keiter, Harper Collins College Publisher, New York,1993.
2. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and C.H. Langford, ELBS, Oxford University Press,2000.
3. Inorganic Chemistry, G.L.Miessler and D.A.Tarr, Pearson, Delhi,2009.
4. Principles of Organometallic Chemistry, P.Powell, Chapman and Hall, London,1988.
5. Concepts and Models of Inorganic Chemistry, B.Douglas, D.H. McDaniel and J.J. Alexander, John Wiley & Sons, New Delhi,2001.

21CHEP0313 Organic Chemistry – III (3 credits)

Objectives: The objective of the course is to understand stereochemistry of various organic compounds and synthetic uses of selected organic reagents. To know various strategies used in retro synthetic analysis, the basic principles involved in mass spectrometry and also combined spectroscopy problems involving simple organic molecules. To understand the chemistry of selected alkaloids.

Course outcome: At the end of the course, students will be able to:

- *Assign R/S and E/Z nomenclature and analyze asymmetric synthesis and topical relationship in organic molecules.*
- *Assess the mechanism and synthetic uses of selected reagents and reactions.*
- *Describe the important concepts of the organic chemistry for the synthesis of new molecule, introduction of different functional group.*
- *Interpret mass spectral data Analyze and identify simple organic molecules by using UV, IR, Mass, ^{1}H NMR and ^{13}C NMR data.*
- *Elucidate the structure and plan for the synthesis of selected alkaloids.*

Unit I –Stereochemistry

R/S system on nomenclature of central and axially chiral molecules – atropisomerism, isomerism of biphenyls, allenes, spiranes, paracyclophanes and ANSA compounds – Geometrical isomerism – E/Z nomenclature – determination of configuration of geometrical isomers – asymmetric synthesis – substrate controlled methods, auxillary controlled methods, reagent controlled methods and catalyst controlled methods – chiral catalyst – Cram's rule – Prelog's rule.

Topical relationship in organic molecules – Homotopic, enantiotopic, diastereotopic groups and faces, Pro R and S descriptors and Re and Si for ligands.

Unit II - Organic Reagents-II

Study of synthetic applications of the following reagents –n-BuLi, Et_2Zn, CBS-catalyst, EDCI, DCC, HATU, HOBT, CAN, TEMPO and IBX.

Unit III - Strategies in Organic Synthesis

An introduction of synthons and synthetic equivalents, disconnection approach, functional group interconversion of halides, nitriles, azides, amines, and esters -the importance of order of events in organic synthesis, nucleophilic and electrophilic synthons - umpolong reactions - typical examples of one group C-X and two group C-X disconnections – two group disconnections – 1,2-difunctionalised compounds – 1,3- -

α, β-unsaturated carbonyl compounds – 1,4-difuctionalised compounds – Diels – Alder reactions and Micheal additions.

Unit IV – Mass Spectrometry and combined spectroscopic problems

Mass spectrometry: resolution – EI and CI methods – basic peak, isotopic peaks, meta-stable peak, parent peak, determination and use of molecular formula – recognition of molecular ion peak – fragmentations – general rules – pattern of fragmentation for various classes of compounds – McLafferty rearrangement – use of meta-stable peaks. Combined spectroscopy problems involving simple organic molecules and UV, IR, NMR and MS data.

Unit V – Alkaloids

Structural elucidation and synthesis of following alkaloids: atropine, quinine, reserpine and morphine.

References:

1. A. J. Kirby, Stereoelectronic Effects, Oxford University Press, 1996.
2. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds Wiley Student Edition, 2008.
3. G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006.
4. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4th edition Cambridge University Press.
5. E. J. Corey and X. M. Cheng, The Logics of Chemical Synthesis, Wiley, 1989.
6. K. C. Nicolaou, Classics in Total Synthesis, Vol 1, 2 and 3.
7. S. Warren and P. Wyatt, Organic Synthesis: The Disconnection Approach, 2nd edition, Wiley, 2008.
8. J. H. Fuhrhop, G. Li, Organic Synthesis: Concepts and Methods, 3rd edition, VCH, 1994.
9. W. Carruthers, Some Methods of Organic Synthesis, Cambridge University Press.
10. H. O. House, Modern Synthetic Reactions, Benjamin-Cummings Publishing Co. 2nd edition, 1972
11. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spectrometric identification of organic compounds, 7th edition, John Wiley, 2005.
12. Organic Spectroscopy, W. Kemp, 3rd edition, Macmillan, 2011.
13. D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, McGraw Hill, 6th edition 2007.
14. D. L. Pavia and G. M. Lampman Spectroscopy 4th Edition, Brooks Cole, 2012.
15. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2004.
16. I.L. Finar, Organic Chemistry, Vol.2 ELBS, 5th edition, 1974 and Pearson India, 5th edition, 2011.

21CHEP0314 Physical Chemistry–III (3credits)

Objectives: Theo bjectiveofthecourseistounderstandthetheoriesofmicrowave,FT-IR,Raman,NMR, ESR and Mossbauer spectroscopic techniques, to know the principle and applications of molecular spectroscopy, and to understand the reactions at the solid surfaces.

Course outcome: At the end of the course, students will be able to:

- *Describe the different theoretical aspects of spectroscopic techniques*
- *Identify the different photophysical processes*
- *Describe and evaluate the application of NMR and ESR techniques to different molecules.*
- *Explain the principle and instrumentation of surface characterization*.

Unit I - Molecular Spectroscopy I

Microwave spectroscopy: Rotation of molecules-Diatomic molecules- rigid and non-rigid rotators-intensities of spectral lines-effect of isotopic dilution-Polyatomic molecules-symmetric and asymmetric Top molecules-chemical analysis by microwave spectroscopy. FT - IR spectroscopy-theory- fundamental vibrations of diatomic and polyatomic molecules-classical theory of Raman effect, Rotational Raman spectra and vibrational Raman spectra.

Unit II - Molecular Spectroscopy II

Electronic spectroscopy-Born-Oppenheimer approximation-Franck-Condon principle, dissociation energy and dissociation products -predissociation-re-emission of energy, fluorescence and phosphorescence-photoelectron spectroscopy-basic principles- photoelectron effect, ionization process, photoelectron spectra of simple molecules. Mossbauer spectroscopy-basic principle-isomer shift, quadrupole splitting, magnetic fieldeffect.

Unit III - Molecular Spectroscopy III

Nuclear magnetic spectroscopy-nuclear spin-nuclear relaxation-magnetic shielding and chemical shift, deshielding, spin-spin interactions-Nuclear Overhauser effect.Introduction to 13C NMR-chemical shift-charge density calculation-broad band decoupling-off resonance decoupling and gated decoupling.Two-dimensional NMR-Basics.

Electron spin resonance spectroscopy-basic principles, hyperfine splitting, zero field splitting and Kramer's degeneracy, factors affecting 'g' value.

Unit IV - Surface Chemistry I

Adsorption and free energy changes at interfaces-solid-gas interface -Langmuir, BET isotherms-surface area determination-soluble and insoluble film-solid-liquid interfaces-Gibbs adsorption isotherm-contact angle and wetting-applications of adsorption.Role of surface in catalysis-semiconductor catalysis-n and p-type surfaces-kinetics of bimolecular surface reactions-Langmuir-Hinshel-Wood mechanism, Langmuir Rideal mechanism and Rideal-Eley mechanism.

Unit V-Surface Chemistry II

Electrical aspects of surface chemistry-electrical double layers-Stren and diffuse layers. Zeta potential concept, determination and applications, electrophoresis, electroosmosis, sedimentation and streaming potential-micelles and reverse micelles, macro and micro emulsions.Principle, instrumentation and applications of ESCA, Auger, SEM, TEM, AFM spectroscopy.

References:

1. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill, New York,1962.
2. Molecular Spectroscopy, C.N. Banwell and E.M. Mcash, Tata McGraw Hill, NewDelhi, 1983.
3. Vibrational Spectroscopy, Satyanarayana, New Age International,1997.
4. Physical Chemistry, P.W. Atkins, ELBS Edn.,1998.
5. Physical Chemistry of Surfaces, W. Adamson, John Wiley and Sons, 3rd Edn.,1976.

M.Sc. CHEMISTRY (III SEMESTER)

21 CHEP0315 Inorganic Chemistry Practical–II (2credits)

Objectives: The practical course is designed to acquire skills in inorganic quantitative estimation methods and to get trained in simple quantitative methods of analysis of inorganic compounds.

Course outcome: At the end of the practical course, students will be able to:

- *Estimate the metals and alloys by using quantitative methods.*
- *Analyze the ores and pharmaceutical preparations quantitatively*

1. Gravimetric analysis – Estimation of mixture of copper andnickel
2. Gravimetric analysis – Estimation of mixture of calcium and barium
3. Colorimetric analysis – Estimation of copper
4. Analysis of cement
5. Analysis of alloys (brass and solder)
6. Estimation of calcium and magnesium in plant samples.
7. Preparation and analysis of a coordination complex.
8. Estimation of pharmaceutical preparations (Paracetamol, Cimetidine)
9. Analysis of iron ore.
10. Estimation of Composition of a complex by Job's method.
11. Colorimetric determination of stability constant of a complex
12. Analysis of a fungicide.

References:

1. Vogel's Text book of quantitative Chemical analysis, G.H. Jaffery, J. Bassett, J. Mendhan and R.C. Deeny. ELBS,1997.
2. Analytical Chemistry in Metallurgy, V.I. Posypaiko and N.A. Vasiua, Mir Publisher, Moscow,1984.

M.Sc. CHEMISTRY (III SEMESTER)

21CHEP0316 Organic Chemistry Practical-II (2credits)

Objectives: The practical course is designed to acquire skills in estimation and multistep synthesis by using various organic reactions and to resolve racemic compounds and synthesize of organic compounds using green methods.

Course outcome: At the end of the practical course, students will be able to:

- *Estimate the selected organic compounds, predict FFA, saponification value, iodine value of oil samples and identify the intermediates and organic compounds.*
- *Resolve racemic mixtures, organic compounds and plan for green synthesis and, multi-component synthesis of organic compounds.*

1. Determination of saponification value of edible oil
2. Determination of iodine value of edible oil
3. Determination of FFA of an oil sample
4. Multistep synthesis of organic compounds involving oxidation, reduction, electrophilic substitution, organometallic reagents, radical reactions.
   Resolution of racemic compounds.
   Green synthesis and multi-component synthesis of selected compounds.

References:

1. Vogel's Text Book of Practical Organic Chemistry, Furniss, S. B.; Hannaford, A. J.;Smith, P. W. G.; Tatchell, A. R. Longman Scientific & Technical, 5thEdn., England,1989.
2. Laboratory Manual of Organic Chemistry, Dey and Sitaraman, Allied Publishers, 1992.

M.Sc. CHEMISTRY (III SEMESTER)

21CHEP0317 Mini Project (1credit)

The candidate will be required to submit a report based on the literature survey and preliminary work carried out as a prelude to the M.Sc. dissertation to be submitted at the end of the IV semester. There will be no ESE for this subject. However, the marks will be awarded for CFA on the basis of the report as well as a Viva-Voce examination conducted by a panel of internal examiners.

M.Sc. CHEMISTRY (IV SEMESTER)

21CHEP0418 INORGANIC CHEMISTRY-IV (4credits)

Objectives: The objective of the course is to understand the basics of nuclear chemistry, types of nuclear reactions and its applications, to know the chemistry and reactions of non- aqueous solvents, to learn the basic principle, reactions and applications of photochemical processes and to have an idea about the general characteristics of f-blockelements.

Course outcome: At the end of the course, students will be able to:

- *Describe the basic concepts of nuclear chemistry and types of nuclear reaction.*
- *Predict the chemistry and reactions of non-aqueous solvents.*
- *Describe the photochemical processes of inorganic molecules.*
- *Examine the general characteristics of f- block elements and analyze the electronic and magnetic properties of their complexes*

Unit I - Nuclear Chemistry I

Nuclear models – Shell model – Liquid drop model - Types of radioactive decay – Alpha decay – Theory of alpha decay - The tunnel effect - Beta decay – Types of beta decay - Electron capture - Dirac's theory - Nuclear deexcitation – Artificial radioactivity. Nuclear reactions: Bathe's notation – Types of nuclear reactions - Elastic and inelastic scattering – Cross section - Q value – Transuraniens - Photonuclear reaction - Radioactive capture - Evaporation and spallation – Buckshot hypothesis - Thermonuclear reactions – Nuclear fusion - Nuclear fission – Fission fragments - Mass and charge distribution – Fission energy.

Unit II - Nuclear Chemistry II

Breeder reactor – Counting techniques: G.M., Ionization and Proportional counter. Applications of radioisotopes – Esterification – Friedal Craft's reaction – Structural determination of PCl5 - Solubility of sparingly soluble substance – Isotope dilution analysis – Carbon dating – Thyroiditis - Assessing the volume of blood in a patient - Brain tumor location and bone fracture healing- Optimum use of fertilizers - Control of predatory insects - Prospecting of water and petroleum.

Unit III - Non-aqueous Solvents

Acid-base, Metathetical, Solvolysis and Redox reactions in liquid ammonia - Hydrogen fluoride - Sulphuric acid and acetic acid solvents- Metal-ammonia solutions - Chemical reactions in liquid sulphur dioxide and phosphoryl chloride.

Unit IV - Inorganic Photochemistry

Principle of light absorption – physical and chemical processes –bimolecular reactions- Stern-Volmer relationship- Properties of d-d, d-π*, π - π*and π -d energy states. Photochemical

reactions of metal complexes – substitution- Admson's rules- rearrangement– isomerisation– racemisation– aquation and anation – redox reactions. Rutheniumpolypyridyls - excited state properties – electron transfer and energy transfer quenching reactions – importance of solar energy conversion and storage – cleavage of water using $Ru(bpy)_3^{2+}$, Cadmium sulphide colloidal particles and titanium dioxide semiconductor –$[Ru(edta)H_2O]$ catalyzed ammonia production.

Unit V - Coordination Chemistry of Lanthanides and Actinides

General characteristics of lanthanides-Electronic configuration-Oxidation state-Lanthanide contraction-Lanthanide contraction and its consequences-extraction- ion exchange and solvent extraction methods-Term symbols for Lanthanide ions (Derivation not required)-Factors that mitigate against the formation of lanthanide complexes-Electronic spectra and magnetic properties of lanthanide complexes-Lanthanide complexes as shift reagents-Difference between 4f and 5f orbitals-Comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.

References:

1. Essential of Nuclear Chemistry, H.J. Arnikar, Wiley- Eastern Ltd., Delhi,2001.
2. Nuclear and Radiochemistry, G. Freindlander, J. W. Kennedy, E.S. Macias, and J. M. Miller, John Wiley and Sons, New York,1991.
3. Inorganic Chemistry, 4thEdn, J.E. Huheey, E.A. Keither and R.L. Keiter, Harper Collins College Publisher, New York,1993.
4. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and CH. Langford, ELBS, Oxford University Press,2000.
5. Fundamentals of Photochemistry, K.K.Rohatgi Mukherjee, New Age International Publisher, New Delhi, 2006.

21CHP 0419 ORGANIC CHEMISTRY - IV (4 credits)

Objectives: The objective of the course is to enable students to know various reaction mechanism involving photochemistry and pericyclic reactions. To understand organic synthesis using protection deprotection strategies and green chemistry and also to know the chemistry of steroids and proteins.

Course outcome*: At the end of the course, students will be able to:*

- *Evaluate concerted reactions via FMO and PMO approach, Electrocyclic reactions, cycloadditions and sigmatropic rearrangements..*
- *Formulate the chemistry of protection and de-protection strategies involved in hydroxyl group by ether and ester, carbonyl group, and amino groups and elementary idea of PTC, microwave and sonochemistry.*
- *Describe the chemistry and structure of cholesterol and oxytocin.*

Unit I – Organic Photochemistry

Fundamental concepts, Jablonski diagram – energy transfer – characteristics of photo reactions – photo reductions and photo oxidation – photoreactions of carbonyl compounds – Norrish type I and Norrish type II reactions, di-pi methane rearrangement – photochemistry of arenes, photochemistry of alkenes, cis-trans isomerisation – rearrangements of cyclic , – unsaturated ketones and 2,5-cyclohexadienone – Barton reaction – Paterno Buchi reaction.

Unit II – Pericyclic Reactions

Pericyclic reactions: Concerted reactions – orbital symmetry and correlation diagram approach – FMO and PMO approach, Woodward-Hofmann rules – Electrocyclic reactions (1,3-butadiene-cyclobutene and 1,3,5-hexatriene-cyclohexadiene systems) – cycloadditions [2+2] and [2+4] systems (ethylene-cyclobutane, ethylene and 1,3-butadiene-cyclohexene systems) – selection rules – cycloreversion (reterocycloaddition reactions) – 1,3-dipolar cycloaddition - sigmatropic rearrangements – Sommelet-Hauser, Cope, Fries and Claisen rearrangements.

Unit III-Protection and Deprotection Chemistry in Organic Synthesis

Protection and cleavage of hydroxyl groups (by ethers)-MOM-Cl, MEM-Cl, THP, Allyl, Benzyl, TBDMS,Protection and cleavage of hydroxyl groups (by esters)-Trichloroacetate, Phenoxyacetate, Pivaloate, 2,4,6-trimethylbenzoate; Protection and cleavage of1,2 and 1,3-Diols-methylene dioxy derivative:Methoxymethyleneacetal, ethyledineacetal, cyclic carbonates; Protection and cleavage of carbonyl groups- 1,3-Dioxanes, 1,3-dithianes, 2,4-dinitrophenylhydrazones; Protection and cleavage of Amino groups-Boc, CBz, Fmoc, N-Acetyl, N-Benzyl.

Unit IV – Green chemistry

Green Chemistry: Designing a green synthesis, basic principles of green chemistry- Atom economy-Phase transfer catalyst, crown ethers- synthesis and applications, Quaternary ammonium salts, polymer supported reagents, ionic liquids and principles and applications of Sono chemistry.

Unit V - Steroids and proteins

Chemistry of Cholesterol (Structural Elucidation) – Conversions of cholesterol to Androsterone, Testosterone, Progesterone.

Proteins: Structure of Proteins-End group analysis-Primary, Secondary, Tertiary and Quaternary Structure of protein. Solid peptide synthesis-Merrifield resin-Chemistry and structure of oxytocin.

References:

1. J. D. Coyle, Introduction to Organic Photochemistry, Wiley, 1991.
2. B. Halton, J. M. Coxon, Organic Photochemistry, Cambridge University Press, 2011.
3. S. Sankararaman, Pericyclic Reactions: A Textbook: Reactions, Applications and Theory, Wiley-VCH, 2005.
4. C.H. DePuy and O.L. Chapman, Molecular Reactions and Photochemistry, Prentice-Hall, New Delhi, 1987.
5. Theodora W. Greene and Peter G. M. Wuts Protective Groups in Organic Synthesis:, John Wiley & Sons, Inc.,3rdEdn., 1999.
6. V.K. Ahluwalia, Renu Aggarwal, Organic Synthesis Special Techniques, Narosa publishing House, 2004.
7. I.L. Finar, Organic Chemistry, Vol.2 ELBS, 5th edition, 1974 and Pearson India, 5th edition, 2011.

21CHEP0420 PHYSICAL CHEMISTRY–IV (4credits)

Objectives: The objective of the course is to give an in-depth account of different theories of statistical thermodynamics and chemical kinetics including the fast reactions.

Course outcome: At the end of the course, students will be able to:

- Describe the role of rotational, vibrational and electronic partition functions.
- Apply different statistical methods
- Predict the rate of the reaction and the influence of solvent and ionic strength.
- Analyze fast reactions by flow, flash and NMR methods

Unit I - Statistical Thermodynamics I

Scope of statistical thermodynamics-probability theorem-phase space, microstate and macrostate, configuration, system, assembly and ensemble-different types of ensembles-permutations and combinations, thermodynamic probability, Maxwell-Boltzmann statistics and its limitations. Concept of partition functions, evaluation of translational, rotational, vibrational and electronic partition functions. Sackur-Tetrode equation- thermodynamic properties of monoatomic gases.

Unit II - Statistical Thermodynamics II

Bose-Einstein statistics-Fermi-Dirac statistics-comparison of the three statistics-Application of Fermi-Dirac statistics to electron gas in metal-Application of Bose-Einstein statistics to photon gas-use of partition functions for obtaining thermodynamic functions – GibbsfreeenergyentropyandprobabilityBoltzmannPlanck'sequationstatisticalapproachtothirdlaw ofthermodynamicsandexceptionofthislaw –molar partition function – specific heat of solids – Einstein theory of specific heat – Debye theory

Unit III - Chemical Kinetics I

Theories of reaction rates-Collision theory and transition state theory, Comparison of collision theory with transition state theory, Arrhenius equation- characteristics, Significance of energy of activation, Temperature coefficient and its evaluation. Thermodynamic formulation of absolutereactiontheoryLindeman'stheoryofunimolecularreactions,Marcus theory of electron transfer process.Derivations of rate constants for opposing, consecutive and parallel reactions steady state approximation.

Unit IV - Chemical Kinetics II

Kinetics of reactions involving reactive atoms and free radicals - Rice-Herzfeld mechanism and kinetics of organic gas phase decompositions (acetaldehyde & ethane); Kinetics of chain reactions-branching chain and explosion limits (H_2-O_2 reaction as an example). Factors influencing reaction rate in solution, significance of dielectric constant, salt effect, and kinetic isotope effect. Oscillatory reactions.

Unit V - Chemical Kinetics III

Concept of linear free energy relationships- thermodynamic implications of LFER-Catalysis- kinetics of homogeneously catalyzed reactions, mechanism of acid-base catalysis. Comparison of enzyme catalysed and chemicalcatalysed reactions, Mechanism (Lock and Key theory). Experimental methods for the study of fast reactions-flow method-chemical relaxation methods, T-jump and P-jump methods, ultrasonic absorption techniques, reaction in a flow system, continuous and stopped flow, shock wave tube method. Flash methods-nuclear magnetic resonance method.

References:

1. Physical Chemistry, R. Stephen Berry, S.J. Rice, and J.Ross, 2nd edn., OxfordUniversity press, New York,2000.
2. Chemical Kinetics and Dynamics, J.J. Steinfeld, J.S. Franciso and W.L. Hase, 2nd edn., Prentice Hall, New Jersey, 1999.
3. Physical Chemistry, P. W. Atkins, Oxford University Press,1998.

M.Sc. CHEMISTRY (IV SEMESTER)

21CHEP0421 DISSERTATION (4Credits)

The candidate is required to submit the dissertation based on an experimental/theoretical study undertaken in one of the branches of chemistry on the topic assigned by the Project Supervisor. The CFA will be based on interim report and a presentation before the panel of internal examiners. The ESE will be based on the final report and on the basis of Viva-Voce examination conducted jointly by the external examiner and the project guide.

DISCIPLINE CENTRIC ELECTIVE

21CHEP03D1 POLYMERCHEMISTRY (4 credits)

Objectives: The objective of the course is to stress the importance of polymers, to understand various polymerization techniques and characterization of polymers, to understand polymer structure, properties and to know the polymer processing techniques, and the chemistry of commercially available polymers and polymer additives.

Course outcomes: At the end of the course, students will be able to:

- *Describe the principles and concepts of contemporary polymer chemistry.*
- *Explain the basic concepts of polymer synthetic techniques.*
- *Analyze the basic reactions in polymer chemistry.*
- *Describe the physical properties of different polymers.*
- *Characterize the polymers by using various experimental techniques*

Unit I - Types and Chemistry of Polymerization

Classification of polymers, Types of polymerization – addition, free radical, ionic and coordination polymerization – Ziegler-Natta Catalyst, Stereo regular polymerization, Condensation polymerization – Mechanism and Kinetics of addition and condensation polymerization – degree of polymerization – kinetic chain length – factors affecting chain polymerization- inhibition and retardation – Carother's equation- Polymerisation techniques- bulk, solution, suspension and emulsion polymerization.

Unit II - Copolymerization and Polymerization Techniques

Types of copolymers- ideal, alternating, block and graft copolymer – Types of copolymerization – Free radical ionic copolymerization –polycondensation – copolymer equation – significance – monomer and radical reactivity – Q-e scheme - Determination of monomer reactivity ratio – Mayo-Lewis and Fineman Ross methods – block and graft copolymerization – methods of preparation and mechanism.

Unit III - Polymer Characteristics and Characterization

Types of degradation – thermal, mechanical and photodegradations - Green methods of management of plastics in the environment.

Polymer purification - separation of polymers – precipitation and isolation by gel permeation chromatography. The concept of number average and weight averages. Molecular weight methods - Molecular weight distribution, - determination of molecular weights – Osmotic pressure, light scattering, viscosity and end group analysis, ultra centrifugation methods.

Analysis and testing of polymers- physical / mechanical and chemical analysis of polymers – spectroscopic methods, x-ray diffraction study.

Unit IV - Structure, Properties and Fabrication of Polymers

Morphology and order in crystalline polymers – configurations of polymer chain –types of stereo isomerism in polymer – tacticity (eg. Mono and disubstitute polyethylene, polypropylene, polybutadiene) significance of stereoregularity.

Polymer structure and physical properties – crystalline melting point Tm – melting points of homogeneous series – effect of chain flexibility and heat of fusion. The glass transition temperature, Tg-relationship between Tm and Tg, effects of molecular weight,chemical structure, property requirements and polymer utilization. Fabrications of polymers – Moulding, casting, calendering and spinning of polymers.

Unit V – Chemistry of Commercial Polymers and Polymer Additives

Organic polymers polyethylene, polyvinyl chloride, polytetrafluoroethylene, polyamides, polyesters, phenolic resins, epoxy resins. Dendrimers – Types and applications.poly (organophosphazenes) polymers, Inorganic polymers – silicon polymers, glass, Basic concept of conducting polymers, liquid crystal polymer, biopolymer and biomedical polymer.

Polymer additives: Fillers, plasticizers, colourants, anti oxidants, fire retardants and thermal stabilizers – polymer blends andcomposites.

References:

1. Text book of polymer science, F.W. Billmeyer Jr. 3rdEdn., Wiley, India2007.
2. Polymer science, V.R. Gowarikar, N.V. Viswanathan, New age international,2003.
3. Principles of polymerization, George Odian, 4th Edn., John wiley and sons,2007.
4. Polymer science and technology, Goel R. Fried, Prentice – Hall of India, New delhi, 2000.
5. Polymer science and technology of plastics and rubbers, P. Ghosh, Tata McGraw-Hill, New Delhi,1998.
6. Introductory polymer chemistry, G.S. Misra, Wiley eastern Ltd.,1993.

21CHEP03D2 PHYSICAL ORGANIC CHEMISTRY (4 credits)

Objectives: The objective of the course is to enable students to have an understanding of kinetics of chemical reactions, concepts of solvent effect on reaction rates, the basics of catalysis and correlation analysis.

Course outcome: At the end of the course, students will be able to:

- *Spell out the principles of kinetics.*
- *Identify the solvent effect on reaction rates.*
- *Explain the principle and practice of catalysis.*
- *Describe the basics of correlation analysis and apply it for the reaction mechanism.*

Unit I - Principles of Kinetics

Mechanistic significance of entropy, enthalpy and Gibbs free energy.Arrhenius equation.Transition state theory.Uses of activation parameters.Analogies between kinetics and themodynamics.The concept of transition states.Rapid equilibria among transition states.Reactivity and selectivity principles.

Unit II - Linear free energy relationships

The Hammett equation, substituent constants, interpretation of s-values.Reaction constant.Deviations from Hammett equation.Dual-Parameter correlations, inductive substituent constant. The Taft model, S 1 and SR scales. The Swain-Lupton treatment.The ortho effect.Primary and secondary kinetic isotope effect.Heavy atom isotope effect.Tunneling effect.

Unit III - Principles of Solvent effect

The concept of solvation and preferential solvation.Solvation model.Qualitative theory of the influence of solvent on reaction rate.Thermodynamic measure of solvation.Effects of solvation on reaction rates and equilibria. Various empirical indexes of solvation based on physical properties. Uses of solvation scales in mechanistic studies.Basic concept of solvent isotope effect.

Unit IV - Catalysis

Specific and general catalysis, Acid-base catalysis: General methods of investigation, Mechanisms, Acidity functions and their use in the elucidation of mechanisms Bronsted catalysis law. Enforced and intramolecular acid-base catalysis.Micellar catalysis.

Unit V - Correlation Analysis

Introduction, simple and multiple linear regression, correlation coefficient, t -test, F-test. Criteria of goodness of fit. The relative importance of different effects as indicated by multiple regression. Applications of correlation analysis in understanding reaction mechanisms.

References

1. Kinetics and Mechanisms of Chemical Transformations, J. Rajaram, J.C. Kuriacose, MacMillan India Ltd.,1998.
2. Physical Organic Chemistry, C.D. Ritchise, Marcel Dekker Inc., New York,1990.
3. Physical Organic Chemistry, N.S. Isaacs, Longmann,1998.
4. Correlation Analysis of Organic Reactivity, J.Shorter, Research Studies Press,Chichester, 1998.
5. An introduction to Physical Organic Chemistry, E.M.Kosower,JohnWiley&Sons,New York, 1968.

21CHEP03D3 MEDICINAL CHEMISTRY (4 credits)

Objectives: The objective of the course is to enable students to understand drug actions and to learn chemistry of various types of drugs such as antibiotics, analgesics, antipyretics, cardiovascular,anti-tubercular drugs, antihistamines and antimalarials.

Course outcomes: At the end of the course, students will be able to:

- *Outline the physicochemical properties of drugs.*
- *Describe drug absorption, distribution, metabolism and excretion.*
- *Formulate the synthesis of few important drugs such as analgesics, antipyretics, cardiovascular, anti-tubercular drugs, antihistamines and antimalarials.*

Unit I - Drug action and sulpha drugs

Physiochemical properties in relation to biological action - influence of route of administration. Biotransformation-absorption from stomach -absorption from intestines -sites ofloss -metabolism and excretion, harmful drugs and their side effects. Sulpha drugs - sulphathiazole, sulphamerazine, sulphaguanidine and other sulpha drugs, -synthesis, mechanism of action -uses.

Unit II - Antibiotics

Antibiotics -A study of Chloramphenicol, Penicillin - semisynthetic Penicillin -gross structural features Streptomycin-Cephalasporin and Tetracycline. Polyene antifungal antibiotics-nystatin, fusicidic acid-griesofulvin. (gross structural features not needed).

Unit III - Analgesics and antipyretics

Study of morphine -structure activity relationship (SAR)-morphine analogues-Codeine -synthetic analgesics- pethidines and methadones -narcotic antagonist. Antipyreticanalgesics - salicylic acid, pyrazole and para amino phenol derivatives. Sedatives:Barbiturates, Benzodiazepines.

Unit IV - Cardio Vascular and anti-tubercular drugs

Cardiovascular Drugs -classification, cardiac glysocides, anti-hypertensive and hypotensive agents -mode of action –anti-arythamic agents. Anti -tubercular drugs - sulphanamides -sulphones, p-amino salicylic acid -INH - ethambutal, Rifampicin.

Unit V – Anti-histamines and anti-malarials

Anti-histamines-introduction -mode of action of anti -histamines - SAR -ethylene diamine, ethanol amine, propyl amine and –cyclizine derivatives -synthesis.Anti-malarials-classification -quinine, 4-amino and 8-amino quinolines and pyrimidines.

References:

1. Medicinal Chemistry Vol - I and II, A. Burger, Wiley inter Science, NewYork,1990.
2. Text book of organic, Medicinal and Pharmaceutical Chemistry, O. Wilson, O. Giswoldand F. George, Lippincott Company, Philadelphia, 9thEdn., 1991.
3. Text book of Pharmaceutical Chemistry, Bentley and Driver.

21CHEP03D4 ENVIRONMENTAL CHEMISTRY (4 credits)

Objectives: The objective of the course is to provide an overview of water, air, soil, radioactive and noise pollution including methods for prevention of pollution and its control measures.

Course outcome: At the end of the course, students will be able to:

- *Explain the cause, consequence and cure of various types of pollution.*
- *Identify the effect of metals and metallic compounds on human health.*
- *Assess the implication of climate change.*
- *Describe the methods analyze and control air and water pollution.*

Unit I - Water Pollution

Types of water pollution, ground water and surface water pollution - Sources and harmful effects-sources and effects of major water pollutants-Inorganic pollutants and toxic metals-Oxygen demanding wastes-Organic pollutants-Plant nutrients-detergents-suspended matter-radioactive wastes-Sediments-Thermal pollutants –oilspills – oilspill removal methods-disease causing agents.

Unit II - Air Pollution

Atmo sphere-structure-functions and photochemical reactions-sources of air pollution-Natural and manmade-classification and effects of air pollutants -CO, CO_2, SO_2, SO_3,NO and NO_2- hydrocarbon as pollutant- reactions of hydrocarbons and effects - particulate pollutants-sources and effects of organic and Inorganic particulates - Green house effect -impact on global climate-control measures-role of CFC's -ozone holes-effects of ozone depletion-smog-components of photochemical smog-effects of photochemical smog.

Unit III - Metal Toxicology and Nuclear Pollution

Effects of metals and metallic compounds-sources, toxicology and health risks of iron, arsenic, cadmium, chromium, lead, mercury and nickel. Nuclear pollution-sources-effects of ionizing and non-ionizing radiation - genetic and somatic effects- effects of Cesium-137, Krypton-85 Iodine-131 and Strontium-90 - storage of nuclear wastes-disposal of nuclear wastes-nuclear disasters and their management -some major nuclear accidents.

Unit IV - Pesticides and Soil Pollution

Pesticides-classification, mode of action-toxic effects of chlorinated hydrocarbons, organophosphorous compounds and carbamates-alternatives to chemical pesticides-(pheromones, Juvenile harmones, chemosterilization)-Soil pollutants-sources and effects of industrial wastes-urban wastes-radioactive pollutants-agricultural wastes-solid waste management in cities, soil pollution control measures.

Unit V - Analysis and Control

Sampling of polluted water- preservation-main quality characteristics of water-alkalinity, hardness, total solids- TDS - DO, BOD, COD, TOC, fluoride and chloride. Defluoridation techniques-Iron removal-sampling of gaseous pollutants and particulates – adsorption - absorption - scrubbing – cold trapping – filtration - cyclone separator - gravity settling - electrostatic precipitators - thermal precipitators - analysis of CO by gas chromatography, NO by chemiluminescence and SO_2 by spectrophotometer.

References:

1. Environmental Chemistry, A.K. De, Wiley Eastern Ltd, 3rd Edn.,1994.
2. Environmental Chemistry, B.K. Sharma, Goel Publishers,2001.
3. Environmental Chemistry, M.S. Sethi, Sri Sai Printographers,1994.
4. Text book of Environmental Chemistry, C.D. Tyagi and M.Mehra, Anmol Publishers, 1996.
5. Fundamentals of Environmental Pollution, K. Kannan, S. Chand & Co.,1997.

21CHEP03D5 SUPRAMOLECULAR CHEMISTRY (4 credits)

Objectives: The objective of the course is to provide a concise introduction and applications of supramolecular chemistry.

Course outcome: At the end of the course, students will be able to:

- *Describe about various supramolecular interactions and topological aspects of molecular receptors.*
- *Uses of various analytical methods in supramolecular chemistry.*
- *Identify and design receptors for cationic, anionic and neutral molecules.*
- *Describe about multiple H-bonding interactions used in crystal engineering.*
- *Apply supramolecular chemistry in appropriate fields*

Unit I - Supramolecular interactions and molecular receptors

Supramolecular interactions: Ion-ion, Ion-dipole, dipole-dipole, hydrogen bonding, cation-π, anion-π, π-π, van der Waals interactions. Structural aspects of molecular receptors: Tweezers, crown-ethers, cryptands, carcerands, cucurbit[n]urils, cycophanes, cyclodextrins and calixarenes.

Unit II - Analytical methods in supramolecular chemistry

Studies on supramolecular interactions using ^{1}H-NMR and UV-vis titration techniques, Isothermal Titration Colorimetry (ITC), Crystallography, Dynamic Light Scattering (DLS) and Mass Spectrometry.

Unit III - Molecular recognition of cations, anions and neutral molecules

Molecular recognition of cations by crown-ethers and calixarenes. Molecular recognition of Anions: Anion binding interactions, Challenges in the design of Anion receptors, factors which affect anion complexation, Hofmeister series, examples of neutral tripodal anion receptors and Calixpyrroles as anion receptors. Molecular recognition of Neutral guests - Hamilton's barbiturate receptor, Hunter's quinone, Rebek’s tennis balldimer.

Unit IV - Crystal Engineering Using Multiple Hydrogen Bonds

Language of crystal engineering: supramolecular synthon – hydrogen bond donors and acceptors. Systems Based on DA-AD interactions: Synthons involving Pairs of OH…O, NH…O, OH…N and NH…N hydrogen bonding interactions. Systems based on DD-AA

interactions: Guanidinium nitrate and Guanidinium sulfonates. Systems Based on ADA-DAD Interactions: hexagonal melamine -cyanuric acid hydrogen-bonded array.

Unit V - Applications of supramolecular chemistry

Supramolecular catalysis: Fujita's M4 L6-assembly- unusual [2+2] and [4+2] cycloaddition. Supramolecular polymers - Main chain supramolecular polymers, side-chainsupramolecular polymers, examples of stimuli responsive supramolecular polymers and self-healingpolymers.

References:

1. Supramolecular Chemistry - A Concise Introduction, J. W. Steed and J. L. Atwood, John Wiley,2000.
2. Modern Supramolecular Chemistry-Strategies for Macrocycle Synthesis, Ed: François Diederich, Peter J. Stang and Rik R. Tykwinski, Wiley-VCH Verlag GmbH & Co.,2008.
3. Organic Nanostructures. Ed: Jerry L. Atwood and Jonathan W. Steed, Wiley-VCH Verlag GmbH & Co.,2008.
4. Supramolecular Chemistry of Anions, Ed: Antonio Bianchi, Kristin Bowman James and Enrique Garcia-España, Wiley-VCH1997.
5. Anion Receptor Chemistry. Ed: Jonathan L. Sessler, Philip A. Gale and Won-Seob Cho, RSC Publishing, 2006.
6. Analytical Methods in Supramolecular Chemistry. Ed: Christoph Schalley, Wiley-VCH Verlag GmbH & Co.,2007.
7. Crystal engineering using multiple hydrogen bonds, In Structure and Bonding, Ed: Andrew D. Burrows, Vol. 108, 55-96, 2004.
8. Supramolecular polymers. Ed: Alberto Ciferri, 2nd Edn., CRC Press,2005.

21CHEP03D6 ADVANCED METHODS IN ORGANIC SYNTHESIS (4 credits)

Objectives: The objective of the course is to understand basics of asymmetric synthesis, to know the chemistry of various oxidizing and reducing agents, to understand the reaction and mechanism of selected name reactions, the chemistry of protecting and deprotecting groups and to know the synthesis of selected drug molecules.

Course outcome: At the end of the course, students will be able to:

- *Describe the methods of asymmetric synthesis which involve chiral substrate, chiral reagents, chiral auxiliary and chiral catalyst.*
- *Predict the structure and mechanism of reactions involving selected oxidizing and reducing agents.*
- *Identify the mechanism of selected name reactions.*
- *Analyze the chemistry of protection and de-protection strategies involved in hydroxyl group by ether and ester, carbonyl group, and amino group sand functional group interconversion by substitution reactions.*

Unit I –Asymmetric Synthesis

Basic principles of Asymmetric synthesis – Definition - Stereospecific, Stereoselective – enanatioselective and diastereoselective-Asymmetric synthesis on chiral substrate: Nucleophilic addition to α–chiral carbonyl compounds; Asymmetric synthesis using chiral reagents: Chiral modification of lithium aluminum hydride, BINAL-H - application in reduction of prochiral ketones T. S model; oxazaborolidines. T.S model; Asymmetric Michael addition to α ,β – unsaturated carbonyl compounds T.S model; Asymmetric synthesis using chiral auxiliary: menthol, oxazolidine-2-one, and BINOL; Asymmetric synthesis using chiral catalysts: Sharpless epoxidation. Resolutions via diastereomeric salt formation- Commonly used resolving agents- (S)-phenylethylamine, L-tartaric acid, Resolution of chiral ligands - BINOL, trans1,2-diaminocyclohexane.

Unit II - Oxidation and Reduction reactions

Oxidation : Structure and Mechanism of reactions involving oxidation with PCC, PDC, Swern oxidation, TBHP, DIAD, IBX, Dess-Martine periodinane, TEMPO. Reduction : Structure and Mechanism of reactions involving reduction with BH3:THF, Catecholborane, Na(CN)BH3 , Raney nickel, Zn in acidic media, Lindlar catalyst, Al(OiPr)3, Rosenmund Reduction.

Unit III - Name reactions

Reaction and Mechanism of following name reaction: Arndt-Eistert Syntheis, Buchwald-Hartwig Cross Coupling Reaction, Grubbs reaction, Heck reaction, Suzuki Coupling, Lawesson's Reagent, Mukaiyama Aldol Addition, Sandmeyer Reaction, Stille Coupling, Tebbe Olefination, Yamaguchi Esterification and Robinsonannulations.

Unit IV - Functional Group interconversion by substitution including protection and deprotection

Conversion of Alcohols to Alkylating Agents-Sulfonate Esters, Halides-Introduction of Functional Groups by Nucleophilic Substitution at Saturated Carbon-Nitriles, Oxygen Nucleophiles, Nitrogen Nucleophiles, Sulfur Nucleophiles, Phosphorus Nucleophiles-Interconversion of Carboxylic Acid Derivatives-Acylation of Alcohols, Preparation of Amides- Installation and removal of protective groups-hydroxy protecting groups-Ether-Bn, Tr and PMB-MOM, THP-Silyl-TMS-Cl, TBDMS, TIPS-Cl-Esters-acetic anhydride, benzoyl chloride-Amino-Protecting Groups-Boc, CBz, Bn, Allyl, Phthalyl-Carbonyl-Protecting Groups-1,3- Dioxanes, 1,3-dithianes.

Unit V - Synthesis of Drug molecules

Metabolic drug-Diabetics- Type-1 and Type-2 diabetics-Synthesis of sitaglyptin, Linaglyptin, Saxaglyptin.Proton pump Inhibitors-Synthesis of omeprazole, lansoprazole, pantoprazole. Sulphadrugs –Synthesis of sulphathiazole, sulphamerazine, sulphaguanidine.

References

1. StereochemistryofOrganicCompounds,E.L.Eliel,SamuelH.Wilen,Wiley –IndiaEdition2008.
2. AdvancedOrganicChemistryPartA,F.A.CareyandR.J.Sundberg,Springer,5th Edn.,2007.
3. AdvancedOrganicChemistryPartB,F.A.CareyandR.J.Sundberg,Springer,5th Edn.,2007.
4. Advanced Organic Chemistry Reactions, Mechanisms and Structure, M. B. Smith and J.March, Wiley, 6th Edn., 2007.
5. AGuidebooktoMechanisminOrganicChemistry,P.Sykes,OrientLongman,6th Edn.,1988.
6. Organic Chemistry, I.L. Finar, Vol. II, ELBS, 5th Edn.,1974.
7. ModernMethodsofOrganicSynthesis,Carruthers,W.andColdham,I,CambridgeUniversity Press, UK, 4th Edn.,2004.
8. Organic Synthesis, Michael B Smith, 3rd Edn., Academic Press,2011.
9. ProtectiveGroupsinOrganicSynthesis,TheodoraW.GreeneandPeterG.M.Wuts,3rd Edn., John Wiley & Sons, Inc.1999.
10. Mathad,V.T.;Govindan,S.;Kolla,N.K.;Maddipatla,M.;Sajja,E.;Sundaram,V.;Organic Process Research & Development 2004, 8,266-270.
11. Ahn, K-H.; Kim, H.; Kim, J. R.; Jeong, S. C.; Kang, T. S.; Shin, H. T.; Lim, G. J. Bull. Korean Chem. Soc. 2002, 23,626.
12. Desai, A. A. Angew. Chem. Int. Ed. 2011, 50, 1974 – 1976.

21CHEP04M3 GREEN METHODS IN CHEMISTRY (4 credits)

Objectives: The objective of the course is to understand the basics of green chemistry, types of environmental friendly organic reactions and to have an idea about the need of green chemistry.

Course outcome: At the end of the course, students will be able to:

- *Explain the importance of green chemistry*
- *Demonstrate the basic principles of green chemistry*
- *Examine the general difference between the ordinary type of reactions and green chemistry*

Unit-I: Introduction to green chemistry

What is Green Chemistry? -Need for Green Chemistry-Goals of Green Chemistry-Advantages-Limitations/Obstacles in the pursuit of the goals of Green Chemistry--Basic principles of Green Chemistry-Atom-economy-Rearrangement reactions-Claisen and Fries-Addition reaction-Addition of HBr to alkene-Michel addition-Diels-Alder reaction-reducing toxicity-green solvents.

Unit-II: Microwave Assisted organic synthesis (MAOS)

Microwave activation – advantage of microwave exposure – specific effects of microwave-Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzamide, methylbenzoate to benzoic acid), Oxidation (of toluene, alcohols)-Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Diels-Alder Reaction, Decarboxylation-Microwave assisted solid state reactions: Deacetylation, Deprotection, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; benzimidazoles.

Unit-III: Ionic liquids and PTC

Introduction – synthesis of ionic liquids – physical properties – applications in alkylation **–** hydroformylations– epoxidations – synthesis of ethers – Friedel-craft reactions – Diels-Alder reactions – Knoevengal condensations – Wittig reactions – Phase transfer catalyst - Synthesis – applications of Quaternary ammoniumsalts.

Unit-IV: Ultrasound Assisted organic synthesis (UAOS)

Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizaro reaction, Strecker synthesis, Reformatsky reaction.

Unit V: Organic Reactions in Aqueous media

Organic reactions in water: Acid catalyst (Lewis acid catalyst)-Metal mediated C-C bond formation-(Allylation, Benzylation and Arylation of carbonyl compounds, Aldol, Pinacol coupling-Conjugate addition -1,3-dipolar reactions-triazole and tetrazole ring formation-Reduction of epoxides and halides-Hydroxylation,Bayer-villigeroxidation).

References:-

1. Green Chemistry-An Introductory Text; Mike Lancater; RSC publishers2011.
2. Anastas, P.T. & Warner, J.K. *Green Chemistry-Theory and Practical*, Oxford University Press(1998).
3. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers (2005).
4. Green Chemistry – Environmentally benign reactions – V. K. Ahluwalia. Ane Books India (Publisher).(2006).
5. Green Chemistry – Designing Chemistry for the Environment – edited by Paul T. Anastas& Tracy C. Williamson. Second Edition,(1998).
6. Green Chemistry – Environment friendly alternatives- edited by RashmiSanghi&M. M. Srivastava, Narora Publishing House, (2003).
7. Organic Reactions in Water: Principles,Strategies and Applications-U. M. Lindstrom; Blackwell Publishing Ltd(2007)

GENERIC ELECTIVE COURSE

21CHEP02G1 ELEMENTS OF BIOCHEMISTRY (4 credits)

Objectives: The objective of the course is to provide a comprehensive introduction to biochemistry and to learn the chemistry of enzymes, structures of nucleic acids and biosynthesis of proteins.

Course outcome: At the end of the course, students will be able to:

- *Predict the sources, extraction and purification of enzymes.*
- *Describe the uses of immobilized enzymes.*
- *Analyze the double helical structure of DNA and its replication.*
- *Evaluate the structure of RNA and its transcription*

Unit I - Enzymes

Factors affecting enzyme activity (temperature, pH, substrate concentration, enzyme concentration) active site, enzyme -substrate complex, allosteric interaction, enzyme inhibition, uses of enzymeinhibitors.

Unit II - Enzyme technology

Use of enzymes, selection of sources of enzymes, enzyme extraction (abrasives, liquid shear, osmotic shock, alkali, detergents, organic solvents, sonication) enzyme purification (removal of nucleic acids, removal of solids, purification and concentration, precipitation, adsorption, phase separation, column chromatography, electrophoresis, dialysis).

Unit III - Enzyme immobilization

Methods of immobilization of enzymes (adsorption, covalent bonding, cross linking; entrapment, encapasulation), applications of immobilized enzyme systems, effect of immobilization on Km, V max, the effect of pH and the effect of inhibitors.

Unit IV - DNA and RNA

Double helical structure of DNA, structure of RNA, DNA replication, semi-conservative nature of replication, RNA transcription, Genetic code and biosynthesis of proteins.

Unit V - Recombinant DNA

Cloning vectors, restriction enzymes for cloning, techniques of restriction mapping, construction of a restriction map, construction of chimeric DNA, molecular probes, construction and screening of genomic and CDNA libraries.

References:

1. Biotechnology, M.D. Travan, S. Boffev, Tata McGraw Hill, 1st Edn.,1987.
2. Elements of Biotechnology, P.K. Gupta, Rastogi Publications, 1stEdn.,1994.
3. Biotechnology, K. Trehan, Wiley Eastern Ltd., 1stEdn.,1990.
4. Biochemistry, S.C. Rastogi, Tata Mc.Graw Hill, 1st Edn.,1993.
5. Outlines of Biochemistry, E.E. Conn, P.K. Stumpf, Wiley Eastern Ltd., 4th Edn.,1976.

21CHEP02G2 INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS (4credits)

Objectives: The objective of the course is to develop knowledge in instrumental methods of chemical analysis, to learn the importance of statistical treatment of analytical data, and to understand basic principles, instrumentation and simple applications of spectrochemical,electrochemical, polarimetric, thermal and radiometric techniques.

Course outcome: At the end of the course, students will be able to:

- *Analyze the experimental data and present it systematically.*
- *Describe and adopt suitable separation techniques.*
- *Identify and assess quantitatively using various spectrochemical and electrochemical methodsandwhattechniqueshouldbeusedfortheanalysistosolveaparticularproblem.*
- *Predict the physical and chemical principles upon which the analytical measurement is based.*

Unit I - Statistical Treatment of Analytical Data

Accuracy and precision-significant figures-errors-types of errors-absolute and relative error-mean and relative mean deviations-standard deviation-student's t-test.

Unit II - Theoretical Principles

Basic idea of law of mass action-Le Chatelier principle-the dissociation theory-common ion effect-solubility product -pH scale and buffer solution and buffer action. Problems based on pH and buffer.

Unit III - Separation Techniques

Solvent extraction-ion-exchange method-principle of chromatography-column, thin layer and gas chromatography-principle methodology and simple applications-elementary idea about HPLC.

Unit IV – Spectrochemical Techniques

Absorption of light - Beer's law - UV-Visible and IR spectrophotometry - principle, instrumentation and simple applications.

Unit V - Electroanalytical, Polarimetry, Thermal and Radiometric Techniques

Basic principles and instrumentation of potentiometry, polarimetry and thermogravimetry-simple applications. Principle, instrumentation and simple applications of radiometric titrations-activation.

References

1. Instrumental methods of chemical analysis, G. Chatwal and S. Anand, Himalaya Publishing House, New Delhi,1999.
2. Instrumental Methods of Analysis, H.W. Willard, L.I. Merrit, J.A. Dean and P.A. Settle, CBS Publishers, 7thEdn., 1996.

21CHEP02G3 POLLUTION AND ITS CONTROL MEASURES (4 credits)

Objectives: The objective of the course is to provide comprehensive introduction to pollution of air, water, noise and nuclear pollution. In addition, the course also deals with pollutants and their impact on global environment and human health.

Course outcome: At the end of the course, students will be able to:

- *Identify pollutants and their effect on environment and human health.*
- *Describe the analytical methods to determine water and air quality parameters.*
- *Propose water treatment methods for domestic and industrial purposes.*

Unit I – Air Pollution

Major regions of the atmosphere – composition of air – specific air pollutants and their effects – CO, CO_2, SO_2, SO_3, NO and NO_2 – ozone depletion – acid rain – photochemical smog.

Unit II – Water pollution

Criteria for potable water – major water pollutants – organic, inorganic, heavy metals – (As, Cr, Fe, Pb, Cd, Hg) oil spills – sources – effects.

Unit III – Soil and Pesticide Pollution

Sources, effects of various oil pollutants – pesticides – classification. Toxicity of DDT, BHC, malathion, parathion, carbamates. Alternative sources for pesticides.

Unit IV – Noise and Nuclear Pollution

Noise pollution – sources and effects – nuclear pollution – genetic and somatic effects **–** nuclear disasters and major accidents.

Unit V – Analysis and control methods

Sampling of air and water pollutants – analysis of DO, BOD, COD and TOC in water – Analysis of CO by GC, NO by chemiluminescence and CO_2 by spectrometry.Treatment of water for domestic and industrial purpose – primary, secondary and tertiary treatment methods.

References

1. Environmental Chemistry, A. K. De, 5thedn., New Age International Publisher,2005.
2. Environmental Chemistry, B. K. Sharma, 11thedn., Krishna Prakashan Media Limited, 2007.

MODULAR COURSES

21CHEP03M1 ADVANCED FUNCTIONAL MATERIALS (2 Credits)

Objectives: The objective of the course is to provide a comprehensive introduction of molecular –level devices, machines, to understand the structural and biological properties of dendrimers, to understand the principles of high temperature superconductors, to understand the importance of biodegradable polymers and to understand the principles and concepts of smart polymers.

Course outcomes: At the end of the course, students will be able to:

- *Describe the molecular-level devices and machines.*
- *Predict molecular devices based on various supramolecular interactions.*
- *Propose the synthesis, characterization and application of PAMAM dendrimers.*
- *Identify the structure and importance of various biodegradable polymers, supramolecular polymers and self-healing polymers.*

Unit I – Molecular Level Devices-I

Supramolecular interactions – Molecular machines in biological systems –Introduction to synthetic molecular machines

Unit II –Molecular Level Devices-II

Mechanically interlocked molecules – Pseudorotaxanes – Rotaxanes – Catenanes – Molecular shuttles – Molecular Pumps – Molecular muscles

Unit III –Dendrimers Poly(amidoamine) Dendrimer-Based Multifunctional Nanoparticles

Introduction to dendrimers – Synthesis of dendrimers – convergent synthesis – divergent synthesis - PAMAM Dendrimers: Structure and biological properties

Unit IV - Biodegradable Polymers

Biodegradable polymers - poly -caprolactone- modified poly -caprolactone copolymer with ester, amide and urethane linkages, polyglycolate, polymandelic acid - biodegradable polyamides – polyester urea – polyamide urethane.

Unit V - Smart polymers

Supramolecular polymers - Main chain supramolecular polymers, side-chain supramolecular polymers, examples of stimuli responsive supramolecular polymers, self-healing polymers.

References:

1. Molecular-Level Devices and Machines, In Stimulating Concepts in Chemistry, Ed., Fritz Vögtle, J. Fraser Stoddart and Masakatsu Shibasaki, pp 255-266, Wiley-VCH Verlag GmbH, Weinheim,2000.
2. Poly(amidoamine) Dendrimer-Based Multifunctional Nanoparticles, In Nanobiotechnology II, Ed: Chad A. Mirkin and Christof M. Niemeyer, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim,2007.
3. Polymers and Ecological problems, Ed., J. Guillet, Plenum Press, New York,1973.
4. Polymer Degradation – Principles and Practical Applications, W. Schnabel, Hanser International,1981.
5. Self-Healing Polymers via Supramolecular, Hydrogen-Bonded Networks, in Self-healing Polymers: From principles to applications, Ed: Wolfgang H. Binder, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany,2013.

21CHEP03M2 NANOTECHNOLOGY AND ITS APPLICATIONS (2 Credits)

Objectives: The objective of the course is to enable students to get an introductory idea of some of the fundamentals and current state –of -the art of nanotechnology and to get familiarize with the synthesis, characterization and applications of nanomaterials.

Course outcome: At the end of the course, students will be able to:

- *Appreciate the state of the art developments in the field of nanotechnology.*
- *Identify common themes across nanotechnology.*
- *Predict the major properties of nanoobjects such as nanotubes, quantum dots and nanoparticles.*

Unit I - Introduction to Nanoscience

Definition of terms-nanoscale, nanomaterials, nanoscience, nanotechnology-scale of materials natural and manmade-nanoscience practiced during ancient and modern periods-contributors to the field of nanoscience.

Unit II - Synthesis of Nanomaterials

Top down and bottom up approaches-synthesis of carbon nanotubes, quantum dots, gold and silver nanoparticles.

Unit III - Characterization of Nanomaterials

Electron microscopy techniques-scanning electron microscopy, transmission electron microscopy and atomic force microscopy.

Unit IV - Application of Nanomaterials

Solar cells-smart materials-molecular electronics-biosensors-drug delivery and therapy-detection of cancerouscells.

Unit V - Nanotechnology inNature

The science behind the nanotechnology in lotus effect-selfcleaning property of lotus- gecko footclimbing ability of geckos-water strider-antiwetting property of water striders-spider silkmechanical properties of the spider silk.

References:

1. Nano: The Essentials: Understanding Nanoscience and Nanotechnology, T. Pradeep, McGraw-Hill Professional Publishing,2008.
2. Introduction to Nanoscience, J. Dutta, H.F. Tibbals and G.L. Hornyak, CRC press, Boca Raton,2008.

21CHEP04M1 MOLECULAR ELECTRONICS AND ORGANIC PHOTOVOLTAICS

(2 credits)

Objectives: The objective of the course is to get an introductory idea of molecular electronics, to know about molecular devices and their functions, to learn the methods to fabricate and probe molecular devices and to understand the basics of organic photovoltaics.

Course outcome: At the end of the course, students will be able to:

- *Describe the basics of molecular electronics.*
- *Plan for the fabrication of molecular devices.*
- *Identify the methods of probing individual molecules.*

Unit I - Molecular Electronics – I

Conventional electronics and Its boundaries - Transistor development and Moore's Law- Definition of molecular electronics- -Molecular connectivity- Self assembling techniques.

Unit II- Molecular Electronics – I

Molecular devices: Molecular rectifiers-Molecular resistor-Molecular diode-Three terminal devices - Molecular transistor-Molecular single electron transistor-Molecular wires. Molecular memory devices and data Storage - Molecular switches –Optoelectronic devices.

Unit III- Molecular Electronics - III

Logic devices-Tools and methods to build and probe molecular devices- Break-junction technique- Forming nanogaps with electromigration.

Unit IV - Molecular Electronics - IV

Probing individual molecules- Contact resistance vs. quantized conductance. Integration strategies: Defect tolerance and new molecular architectures.

Unit V- Organic Photovoltaics

Basics of organic solar cells – types of organic solar cells –heterojunction – bulk heterojunction - components of organic solar cells - light absorbing materials – p-i-n concept – tandem cells - cell fabrications. Dye sensitized solar cells -history – operational principles - absorption of light bymolecules.

References:

1. Molecular Electronics - Commercial Insights, Chemistry, Devices, Architectureand Programming by James M Tour,2003, First Edition, World Scientific Publishing Company,Singapore.
2. Molecular Electronics - An Introduction to Theory and Experiment by Juan Carlos Cuevas and ElkeScheer, 2010, First Edition, World Scientific Publishing Company, Singapore.
3. Introducing Molecular Electronics by Cuniberti, Gianaurelio, Fagas, Giorgos, Richter, Klaus (Eds.), 2005, Springer Publishing, Chennai.
4. Third Generation Photovoltaics Advanced Solar Energy Conversion, Martin A. Green, Springer, 1st ed.2003.

21CHEP04M2 WATER QUALITY MONITORING, MANAGEMENT AND TREATMENT

(2 credits)

Objectives: The objective of the course is to given an in-depth understanding of ground water and surface water pollution and its control measures. In addition, the students will also learn the water treatment methods, water analysis methods, sewage and industrial effluent treatment methods and water resource management.

Course outcomes: At the end of the course, students will be able to:

- *Analyze polluted water samples.*
- *Evaluate pollutants and their effect on environment and human health Suggest water treatment methods for domestic and industrial purposes.*
- *Describe the principles and design suitable water treatment processes, including sedimentation, coagulation, chlorination and ozonation as well as sewage and industrial effluent treatment.*

Unit I - Water quality parameters and their determination

Physical, chemical and biological standards significance of these contaminants over the quality and their determinations - Electrical conductivity - turbidity - pH, total solids, TDS - alkalinity - hardness - chlorides - DO - BOD- COD - TOC - nitrate –sulphate-- arsenic - mercury - biomass and chlorophyll estimation - estimation of MPN – bioassay.

Unit II- Water pollution Sources and control measures

Surface and ground water pollution - Harmful effects-pollution of major rivers - protecting ground water from pollution - ground water pollution due to Fluoride, Iron, Chromium and Arsenic sources, ill effects and treatment methods.

Water pollution control- stabilization of the ecosystem – waste treatment reclamation - various approaches to prevent and control water pollution.

Unit III- Water treatment methods

Treatment for community supply - screening, sedimentation, coagulation, filtration - removal of micro organisms - chlorination, adding bleaching powder, UV irradiation and ozonation. Demineralization of water for industrial purposes - boiler problems - scale and sludge formation - prevention of scale formation-internal and external treatment – Demineralization - zeolite process.

Unit IV - Sewage and industrial effluent treatment

Sewage - characteristics - purpose of sewage treatment - methods of sewage treatment - primary - secondary and tertiary - Role of algae in sewage treatment.

Types of industrial wastes - treatment of effluents with organic and inorganic impurities - treatment of waste waters from specific industries - pulp and paper - chemical industry - food processing-water hyacinth in the treatment of industrialeffluents.

Unit V - Water Management

Water resources management - rain water harvesting methods - percolation ponds - check darns - roof top collection methods - water management in industries - recycling and reuse of waste water - metal recovery from metal bearing waste water - recovery of zinc and nickel.

References

1. Chemical and Biological Methods for Water Pollution Studies, R.K. Trivedy andP.K. Goel, Environmental Publications,1986.
2. Engineering Chemistry, P.C. Jain and Monica Jain, Dhanpat Rai & Sons,1993.
3. Environmental Chemistry, B.K. Sharma, Goel Publishing House,2001.
4. Water Quality and Defluoridation Techniques, Rajiv Gandhi National Drinking Water Mission Publication, 1994.

21CHEPO2VS1 DESIGN THINKING INNOVATION AND PRODUCT DEVELOPMENT (2Credits)

Course Objectives

- *Study a problem from multiple perspectives*
- *Learn how to frame the design challenge properly*
- *Learn how to ideate, prototype and Iterate solutions.*
- *Learn from the overall design process how to create value as entrepreneurs*
- *Learn how to design successful products or enterprises.*

UNIT I:

Design *vs.* Design thinking; Design thinking: Understanding the Mindsets-Empathy, Optimism, Embrace Ambiguity, Make it, Learn from Failure, Iterate, Create Confidence, Creativity Convergent & Divergent Thinking. The 5 stages of the Design Thinking process-Empathize, Define (the problem), Ideate, Prototype, and Test.

UNIT II:

Ideation tools & exercises. Sample Design Challenge, Introduction to the Design Challenge-Themes, Storytelling and Tools for Innovation. Empathize-Understand customers, Empathy Maps, Empathize-step into customers shoes- Customer Journey Maps, Define – Analysis & Drawing Inferences from Research.

UNIT III:

The Design Challenge: Define the Design Challenge, Prototyping & Iteration-Feasibility Study, Testing- Documentation and the Pitch.

UNIT IV:

Entrepreneur – Scope; Popular Women Entrepreneurs, Institutional support for entrepreneurs, Start-ups – Development Phases, Preparation of project report, Entrepreneurship *vs.* Startups, SME's *vs*. Scaleups. Opportunities for Startups in India.

UNIT V:

IPR- Genesis and Development, Basic Concepts and Need, Nature- Patents-Patent search, Patent filing, Copyrights, Geographical Indications, trademark, Industrial design; Pros and cons of IPR.

Reference Books

1. Transforming an Idea into a Business with Design Thinking, Mashhood Alam, Routledge, Taylor& Francis Group, USA and UK, 2019

2. Design Thinking, Gavin Ambrose, Paul Harris, AVA Book Production Pvt. Limited.; Singapore, 2010

3. Entrepreneurship & Innovation: Global insights from 24 leaders, James C. Barrood, Rothman Institute of Entrepreneurship, Farleigh Dickinson University, US, 2010

4. Intellectual Property, Siva Vaidhyanathan, Oxford University Press, USA, 2017.

5. Entrepreneurial Development, Jayashree Suresh, Margham Publications , Chennai, 2017.

21CHEPO2VS2 COMPUTING TOOLS IN CHEMISTRY (2 credits)

Objectives: The objective of the course is to learn open source drawing and molecular visualization tools which are necessary for chemists.

Course outcomes: After successful completion of the course, students will be able to

- *Draw molecular structures*
- *Convert 2D molecular structures to 3D structure and perform structure optimization*
- *Visualize molecules and create animations*
- *Analyze single crystal X-ray crystallographic structure and generate images*
- *Interpret 1D and 2D NMR spectral data*

Unit I: Drawing tools in chemistry

Free open-source drawing tools in chemistry: Drawing rings and chains– editing - manipulating the structure – converting to 3D structures – optimizing the structures – graphics

Unit II: 3D molecular visualization tools

Avogadro: Draw – manipulate – measurement of bond angle, bond length – rotation of bonds - Energy minimization – Conformations – visualizing proteins - Animation and graphics

Unit III: Mercury 3.8 (CCDC)

Analyzing single crystal X-ray crystallographic data – measurement of bond angle, bond length and dihedral angle - simulating powder XRD data from single crystal X-ray data – generating graphics – visualizing protein structures

Unit IV: NMR software

Processing ^{1}H NMR and ^{13}C NMR spectra; Integration; peak picking; stacking; interpretation of 2D NMR data – COSY – NOESY.

Unit V: Graphing tools

Graphing tools used in chemistry – plotting graphs – curve fitting analysis – exporting data and graphs – creating graphics

E-resources:

1. https://courseupload.net/chemdraw-professional-maste200321/
2. http://avogadro.cc/
3. https://www.ccdc.cam.ac.uk/solutions/csd-core/components/mercury/
4. https://mestrelab.com/download/mnova/
5. https://www.bruker.com/en/products-and-solutions/mr/nmr-software/topspin.html

21CHEPO2VS3 MATERIALS FOR BIOLOGICAL APPLICATIONS

(2Credits)

Objectives: This course is designed to understand the requirements and to gain insight in to the applications of materials for biological applications.

Course outcome: After successful completion of the course, students will be able to

- *Predict the basic requirements of materials for biological applications*
- *Identify materials for drug and nucleic acid delivery.*
- *Understand the concepts behind smart sensor fabrication.*

Unit – I Design and Preparation of Bio mimetic and Bio inspired Materials

Biocompatibility of materials – materials of biological origin – synthetic materials – surface modification of materials for specific applications - biosorption.

Unit-II Drug Delivery

Types of drug carries - Lipid-based systems - Peptide-based systems -Glycan-based systems -Nucleic acid-based systems – Dendrimer - based systems.

Unit –III Bone Regeneration

Injectable hydrogels as bone regeneration material - Ceramics -Synthetic bone substitute. Wound healing Therapeutic protein - Growth factor.

Unit – IV Smart Devices

Sensor – Sensing principles - Transducer - Electronic tongues and aptasensors Electrochemical sensor arrays - Electronic tongue – Aptasensors – Potentiometry Voltammetry – Biomarkers - Biomedical applications - Pharmaceutical applications. Smart devices - Smart stent – Optrodes. Organ-on-chip. Microfluidics – On-chip integration – Detection-Diagnosis.

Unit – V Nucleic Acid Delivery

Gene delivery - Nonviral vectors - Lipid-based vector - Polymer-based vector - siRNA-conjugates. Artificial virus particles Virus-like particles - Viral nanoparticles – Bacteriophages - Genetic engineering - Chemical modifications - Biomedical applications.

References:

1. Bioinspired Materials for Medical Applications by *L. Rodrigues and M. Mota Woodhead Publishing 2017.*
2. Biological Materials Science: Biological Materials, Bioinspired Materials, and Biomaterials, by **M. A. Meyers and P-Y. Chen,** Cambridge University Press, 1st ed. 2014.
3. Engineered Carbohydrate-Based Materials for Biomedical Applications: Polymers, Surfaces, Dendrimers, Nanoparticles, and Hydrogels by R. Narain, John Wiley & Sons,

21CHEP04VS4 HUMAN VALUES AND PROFESSIONAL ETHICS

Objectives: This course is designed to understand the human values, ethics, quality control to understand the ethical responsibilities.

Course outcome: On completion of this course, the students will be able to

- ➢ *Understand the significance of human values.*
- ➢ *To Understand the safety responsibilities of occupation.*
- ➢ *To Know the good practice of manufacturing in pharma industries.*
- ➢ *To Understand the values and science in ethics.*

Unit I - Human Values

Objectives, Morals, Values, Ethics, Integrity, Work Ethics, Service Learning, Virtues, Respect For Others, Living Peacefully, Caring Sharing, Honesty, Courage, Valuing time, Co-Operation, Commitment, Empathy, Self - Confidence, Challenges in the workplace, Spirituality.

Unit 2 - Safety, Responsibility and Rights

Safety definition, Safety and Risk, Risk analysis, Assessment of safety and risks, Safe exit, Risk benefit analysis, Safety lesson from challenges, Collective bargaining, Confidentiality, Conflict of interest, Occupational crime, Human rights, Employee rights, Whistle Blowing, Intellectual property rights.

Unit 3 - Introduction to GMPs

Quality assurance and related concepts, GMP - a concept, Sanitation and hygiene, Quantification and validations, Complains, Products recalls, Contract production and analysis, Self-inspection, Quality audits, Supplier audits and approvals, Training, personal hygiene, Equipments, materials and documentations.

Unit 4 - Practice of GMPs

Good practice in production, Good practice in quality control, Good manufacturing practice for APIs (Bulk drug substances), Supporting and supplementary guidelines for sterile products.

Unit 5 - Values and Science

Introduction, Scientists responsibility, scientific responsibility, Ethical responsibility, inadequate behavior of scientists, Ethical valuation, The need of ethics in scientific activity.

References:

1) R.S Naagarazan, A text book on personal ethics and human values, New Age International Publishers, New Delhi.
2) P.P Sharma, How to practice GMPs, 7th Edition, Vandana Publications, New Delhi.
3) J.A.V Matas, Values and Science: An Analysis for The Ethics In Science - A Review Article, Sociology International Journal, **2018**, *2*, 257 - 265.

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