

M.Sc. Chemistry

Syllabus

(with effect from June 2018)

DEPARTMENT OF CHEMISTRY

The Gandhigram Rural Institute – Deemed to be University

Gandhigram – 624 302 TamilNadu

Semester-wise credits distribution for M. Sc. Chemistry-2018

Course code	Title of the Course	Credits	Hours		Max Marks		
			Theory	Practical	CFA	ESE	Total
FIRST SEMESTER							
18CHEP0101	Inorganic Chemistry -I	4	4	-	40	60	100
18CHEP0102	Organic Chemistry – I	4	4	-	40	60	100
18CHEP0103	Physical Chemistry – I	4	4	-	40	60	100
18CHEP0104	Analytical Chemistry	3	3	-	40	60	100
18CHEP0105	OrganicChemistryPractical-I	2	-	5	60	40	100
18CHEP0106	PhysicalChemistryPractical-I	2	-	5	60	40	100
18GTPP0001	Gandhi in Everyday Life	-	2	-	50	-	50 [#]
Total		19	17	10	330	320	650
SECOND SEMESTER							
18CHEP0207	Inorganic Chemistry – II	4	4	-	40	60	100
18CHEP0208	Organic Chemistry – II	4	4	-	40	60	100
18CHEP0209	Physical Chemistry – II	4	4	-	40	60	100
18CHEP0210	InorganicChemistryPractical-I	2	-	5	60	40	100
18CHEP0211	Physical Chemistry Practical– II	2	-	5	60	40	100
*	Non Major Elective	4	4	-	40	60	100
18ENGP00C1	CommunicationAndSoftSkills	-	2	-	50	-	50 [#]
Total		20	18	10	330	320	650

THIRD SEMESTER							
18CHEP0312	Inorganic Chemistry -III	3	3	-	40	60	100
18CHEP0313	Organic Chemistry – III	3	3	-	40	60	100
18CHEP0314	Physical Chemistry – III	3	3	-	40	60	100
18CHEP0315	InorganicChemistryPractical-II	2	-	5	60	40	100
18CHEP0316	OrganicChemistryPractical-II	2	-	5	60	40	100
18CHEP0317	Mini-Project	1	-	-	50	-	50
18CHEP03EX	Major Elective	4	4	-	40	60	100
18CHEP03MX	Modular Course	2	2	-	50	-	50 [#]
18EXNP03V1	VPP	2	-	-	50	-	50 [#]
18CHEP01F1	Extension / Field Visit	2	-	2	-	-	-
Total		24	15	12	430	320	750
FOURTH SEMESTER							
18CHEP0418	Inorganic Chemistry –IV	4	4	-	40	60	100
18CHEP0419	Organic Chemistry – IV	4	4	-	40	60	100
18CHEP0420	Physical Chemistry – IV	4	4	-	40	60	100
18CHEP04MX	Modular Course	2	2	-	50	-	50 [#]
18CHEP0421	Dissertation	6	-	12	75	75+	200
18CHEP01F2	Extension / Field Visit	2	-	2	-	-	-
Total		22	14	14	245	305	550
Grand Total		85	64	46	1335	1265	2600

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

Not included for CGPA calculation

LIST OF MAJOR ELECTIVE COURSES OFFERED (4 credit)

1. 18CHEP03E1 - Polymer Chemistry
2. 18CHEP03E2 - Physical Organic Chemistry
3. 18CHEP03E3 - Medicinal Chemistry
4. 18CHEP03E4 - Environmental Chemistry
5. 18CHEP03E5 - Supramolecular Chemistry
6. 18CHEP03E6 - Advanced Methods in Organic synthesis
7. 18CHEP04M3 - Green Methods in Chemistry

LIST NON MAJOR ELECTIVE COURSES OFFERED (4 credit)

1. 18CHEP02N1 - Elements of Biochemistry
2. 18CHEP02N2 - Instrumental Methods of Chemical Analysis
3. 18CHEP02N3 - Pollution and its Control Measures

LIST OF MODULAR COURSES OFFERED (2 credit)

1. 18CHEP03M1 - Advanced Functional Materials
2. 18CHEP03M2 - Nanotechnology and Its Applications
3. 18CHEP04M1 - Molecular Electronics and Organic Photovoltaics
4. 18CHEP04M2 - Water Quality Monitoring, Management and Treatment

M.Sc. CHEMISTRY (I SEMESTER)

18CHEP0101

Inorganic Chemistry-I

(4 credit)

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 in it.*

Unit I - Bonding Models I

Ionic bond - Lattice energy and determination - Born-Landé 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 of diatomic and triatomic molecules.

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 - Charge distribution in molecules - Dipole moment - Determination and applications.

Unit III – Solid State Chemistry I

Cells and description of crystal structure - 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 and calcite.

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 of solids.

Unit V - Acid-Base Concept

Acid-Base concept- Solvent system concept - 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 – Quantitative measurements – Applications of HSAB theory - Inductive effects - Strength of oxyacids - Pauling's rule - Acidity of cations in aqueous solution- solvation and acid base strength.

Text Books:

1. Text book of Inorganic Chemistry, P. L. Soni, M. Katyal, Sultan Chand and Publishers, 20th revised Edn. 2010.
2. Inorganic Chemistry, J.E. Huheey, E.A. Keither and R.L. Keiter, Harper Collins College Publisher, New York, 4thEdn.,1993.
3. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and CH.Langford, ELBS, Oxford University Press, 6thEdn., 2015.
4. Theoretical Principles of Inorganic Chemistry, GS. Manku, Tata McGraw Hill Publishing Company Ltd., New Delhi,1994.
5. Solid State Chemistry, D.K. Chakrabarthy, New Age International Publishers, NewDelhi, 2005.

Reference Books:

1. Modern Inorganic Chemistry, W.E. Jolly, McGraw Hill International Edition, New York,1994.
 2. Inorganic Chemistry, Gary Wulfsberg, University Science Books, 2000.
 3. Concepts and Models of Inorganic Chemistry, B.Douglas, D.H.Me Daniel and J.J. Alexander, John Wiley and Sons, New Delhi,2001.
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M.Sc. CHEMISTRY (I SEMESTER)

18CHEP0102

Organic Chemistry– I

(4credit)

Objectives: The objective of the course is to develop an understanding of reactivity organic compounds, reaction mechanisms, characterization of organic compounds by UV and IR. The course also will give an understanding of the chemistry of carbohydrates particularly di and tri-saccharide.

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

- Describe inductive effects, field effects, resonance, hydrogen bonding, hyperconjugations and also aromaticity of annulenes, azulenes and ferrocene.
- Assess the thermodynamic and kinetic controlled products and methods of determination of reaction mechanisms.
- Elucidate the structure of organic compounds using UV and IR Identify the mechanism of various photochemical reactions.
- Describe the chemistry of disaccharides, trisaccharides and oxygen heterocycles.

Unit I – Electronic Effects, Aromaticity and Acids and Bases

Electron Displacement – Inductive and field effect – Delocalised bonds – Rules of resonance -steric inhibition of resonance, steric enhancement of resonance, Hyperconjugation – Hydrogen bonding – Intra and inter molecular hydrogen bonding – effect of hydrogen bonding and hyperconjugation on physical and chemical properties. Effect of structure and medium on the strengths of acids and bases. 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 - concept of homoaromaticity.

Unit II – Methods of Determination of Reaction Mechanisms

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 – Taftequation.

Unit III – UV-vis and IR Spectroscopy

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

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

Unit IV – 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- π methane rearrangement – photochemistry of arenes, photochemistry of alkenes, cis-trans isomerisation – rearrangements of cyclic, – unsaturated ketones and 2,5-cyclohexadienone – Barton reaction – PaternoBuchi reaction.

Unit V – 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.

Text Books:

1. A Guide Book to Mechanism in Organic Chemistry, P. Sykes, Orient Longman, 6thEdn., 1988.
2. Spectrometric identification of organic compounds, R.M. Silverstein, F.X. Webster, D.J. Kiemle, 7thEdn., John Wiley & Sons, New Delhi, 2006.
3. Organic Spectroscopy, W. Kemp, ELBS, 2ndEdn., 1991.
4. Organic Chemistry, I.L. Finar, Vol.2 ELBS, 5thEdn., 1974.
5. Molecular Reactions and Photochemistry, C.H. DePuy and O.L. Chapman, Prentice-Hall, New Delhi, 1987.

Reference Books:

6. Advanced Organic Chemistry. Part-A. Structure and Mechanisms, F. Carey, R. Sundberg, 4th Ed., Kluwer Publishers, 2000.
 7. March's Advanced Organic Chemistry, Michael B. Smith, J. March John Wiley & Sons, 6thEdn., 2007.
 8. Organic Chemistry, J. Clayden, N. Greeves, P. Wothers, Oxford University Press, 2001.
 9. Organic Chemistry, J. Mc. Murry, Brooks/Cole publisher, 5thEdn., 2000.
 10. Organic Synthesis, M. B. Smith, Academic Press, Elsevier, 3rdEdn., 2010.
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M.Sc. CHEMISTRY (I SEMESTER)

18CHEP0103

Physical Chemistry-I

(4credit)

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 and the definition of fugacity. 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. Lewis Randal rule-Duhem-Margules equation-Definition of activity and activity coefficient-variations of activity with pressure and temperature-determination of activity and activity coefficient of non-electrolytes.

Unit II - Third Law of Thermodynamics and Chemical Equilibrium

Third law of thermodynamics -purpose-formulations (Plank, Lewis and Randal)-Thermodynamic properties at absolute zero temperature-calculation of absolute entropies-apparent exception to III law.

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 inequality-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

Formation of electrical double layer-electrocapillary curves-Lippmann equation-structure of electrified interfaces-Helmholtz-Perrin model -Gouy-Chapman model -electrode kinetics-derivation of the fundamental equation of electrode kinetics. Butler-Volmer equation-low field and high field approximations-Tafel equation-Electrochemical theory of corrosion-protection from 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. Lead-acid batteries-Cadmium-Nickel oxide batteries-charging and discharging reactions-Fuel cells-classification-chemistry of fuel cells-detailed description. Supercapacitors – types of supercapacitors.

Text Books:

1. Fuel Cells-Principles and Applications, B.Viswanathan, M.AuliceScibioh, Universities Press, Hyderabad, India,2006.
2. Modern Electrochemistry, John M. Bockris and Amulya K.N. Reddy, Vol. I & II, 2ndEdn., Springer, New Delhi,2000.
3. Physical Chemistry, P.W. Atkins, Oxford University Press,1998.
4. Thermodynamics for students of Chemistry, Kuriakose and Rajaram, Shoban Lal Nagin Chand,1986.

Reference Books

1. Electrochemical Methods Fundamentals and Applications, Allen J. Bard and Larry R. Faulkner 2ndEdn., John Wiley and Sons,2004.
 2. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula,Oxford Publishers, 2014.
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M.Sc. CHEMISTRY (I SEMESTER)

15CHEP0104

Analytical Chemistry-I

(3 credit)

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 solvent extraction.

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 (ICP- AES)-principle and applications. XRD-principle-single crystal-powder crystal methods and application.

Unit III - Radiochemical and Thermal Methods of Analysis

Isotopic dilution methods - neutron activation analysis – Radiometric titrations - 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-Ilkovic equation-Half-wave potential-applications. Cyclic voltammetry-interpretation of cyclic voltammogram- principle-simple analytical applications- -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-principle and applications.

Text Books:

1. Principles of Instrumental methods of analysis, Skoog and West, Saunders College Publications, 1992.
2. Instrumental methods of chemical analysis, B.K. Sharma, Goel publishing House, 19thEdn.,2000.
3. Electrochemical Methods, Fundamentals and Applications, A.J. Bard and L.R. Faulkner, John Wiley & Sons, 2ndEdn.,2001.

Reference Books

1. Instrumental methods of analysis, H.W. Willard, L.I. Merrit, J.J.A. Dean and F.A. Settle, CBS publishers,1983.
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15CHEP0105

M.Sc. CHEMISTRY (I SEMESTER)
Organic Chemistry Practical-I

(2 credit)

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.

Text Books:

1. Laboratory Manual of Organic Chemistry, Dey and Sitaraman, Allied Publishers, 1992.
2. Organic Chemistry Lab Manual, N. S. Gnanaprakasam, G. Ramamurthy, S. Viswanathan Printers and Publishers Pvt. Ltd., 2015.

Reference Book

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.
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M.Sc. CHEMISTRY (I SEMESTER)

15CHEP0106

Physical Chemistry Practical-I

(2 credit)

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 ZnSO₄/ KCl / Hg₂Cl₂ / Hg / Ag / AgCl / 0.1 M KCl / Hg₂Cl₂/ Hg/ Hg₂Cl₂/ KCl/ 0.1 M CuSO₄/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 AgNO₃.
 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 CH₃COOH by NaOH.
 11. Determination of solution enthalpy by thermometric method. Oxalic acid-water, K₂Cr₂O₇-water and Naphthalene -toluene.

Text Books:

1. Practical Physical Chemistry, B. Viswanathan and P. S. Raghavan, Viva Books Pvt. Ltd., New Delhi, 2008.
2. Senior Practical Physical Chemistry, D. D. Khosala, A. Khosala, V. C. Gard, R. Chand & Co., New Delhi, 1975.

Reference Books:

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 Kogakusha Ltd., 1970.

M.Sc. CHEMISTRY (II SEMESTER)

18CHEP0207

Inorganic Chemistry– II

(4 credit)

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) – 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 – 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-Factors influencing stability constants.

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 for racemisation.

Unit IV - Coordination Chemistry (Reaction Mechanism II)

Trans-effect - Theories of trans-effect, pi-bonding theory and polarization theory- Application of trans effect-cis effect. Redox 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. Splitting of free ion terms in octahedral field - correlation diagram - Orgel diagrams for d^1 to d^9 ions and Tanabe-Sugano diagrams for d^2 and d^3 ions.

Text Books:

1. Inorganic Chemistry, J.E. Huheey, E.A. Keiter and R.L. Keiter, Harper Collins College Publisher, 4th Edn., New York, 1993.
2. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and C.H. Langford, ELBS, Oxford University Press, 2000.

Reference Books:

1. Inorganic Chemistry, G.L. Miessler and D.A. Tarr, Pearson, Prentice Publishers, Delhi, 2009.
 2. Inorganic Chemistry, B. Douglas, D.H. McDaniel and Concepts and Models of J.J. Alexander, John Wiley and Sons, New Delhi, 2001.
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M.Sc. CHEMISTRY (II SEMESTER)

18CHEP0208

Organic Chemistry– II

(4 credit)

Objectives: The objective of the course is to understand various reaction mechanisms in organic chemistry, to have advanced knowledge in NMR spectroscopy, to know the chemistry of organic molecules based on stereochemistry, to understand the chemistry of photochemical pericyclic reactions and the chemistry of terpenoids.

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

- Describe and formulate the mechanism of various nucleophilic substitution reactions and elimination reactions.
- Interpret the NMR spectra
- Assign R/S and E/Z nomenclature and analyze asymmetric synthesis and topical relationship in organic molecules.
- Evaluate concerted reactions via FMO and PMO approach, Electrocyclic reactions, cycloadditions and sigmatropic rearrangements.
- Elucidate the structure and propose synthesis of selected terpenoids.

Unit I – 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: E_1 , E_2 and E_{1cB} – evidences – effect of structure, solvent and base – Hoffmann and Saytzeff rules – stereochemistry of E_1 reaction – Pyrolytic elimination – cis elimination – elimination vs substitution.

Unit II – NMR Spectroscopy

NMR Spectroscopy: 1H -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, -NH₂) – non 1 order spectra – simplification of complex spectra – double resonance – shift reagents – NOE and its applications.

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

Unit III –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, auxiliary 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 IV – Photochemistry (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 (retrocycloaddition reactions) – 1,3-dipolar cycloaddition - sigmatropic rearrangements – Sommelet-Hauser, Cope, Fries and Claisen rearrangements.

Unit V – Terpenoids

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

Text Books:

1. A Guide Book to Mechanism in Organic Chemistry, P. Sykes, Orient Longman, 6thEdn., 1988.
2. Spectrometric identification of organic compounds, R.M. Silverstein, F.X. Webster, D.J. Kiemle, 7thEdn., John Wiley & Sons, New Delhi, 2006.
3. Organic Spectroscopy, W. Kemp, ELBS, 2ndEdn., 1991.
4. Organic Chemistry, I.L. Finar, Vol.2 ELBS, 5thEdn., 1974.
5. Molecular Reactions and Photochemistry, C.H. DePuy and O.L. Chapman, Prentice-Hall, New Delhi, 1987.
6. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Publishers, 6thEdn., New Delhi, 2005.
7. Stereochemistry of Organic Compounds: Principles and Applications, D. Nasipuri, New Age International Publishers, 2ndEdn., New Delhi, 2005.

Reference Books

1. Advanced Organic Chemistry. Part-A. Structure and Mechanisms, F. Carey, R. Sundberg, 4th Ed., Kluwer Publishers, 2000.
 2. March's Advanced Organic Chemistry, Michael B. Smith, J. March John Wiley & Sons, 6thEdn., 2007.
 3. Organic Chemistry, J. Clayden, N. Greeves, P. Wothers, Oxford University Press, 2001.
 4. Organic Chemistry, J. Mc. Murry, Brooks/Cole publisher, 5thEdn., 2000.
 5. Organic Synthesis, M. B. Smith, Academic Press, Elsevier, 3rdEdn., 2010.
 6. Stereochemistry of Carbon Compounds, E.L. Eliel, McGraw Hill Book Company, New York, 1975.
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M.Sc. CHEMISTRY (II SEMESTER)

18CHEP0209

Physical Chemistry–II

(4 credit)

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 Eigenfunctions.*
- *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-Schrodinger 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 for a rotating diatomic molecule-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 and NO.

Unit IV Basics of Group Theory

Definition of a mathematical group and its properties – group multiplication table - cyclic groups-subgroups - classes – symmetry elements - symmetry operations – classes of symmetry operations - 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- π -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 .

Text Books:

1. Introductory Quantum Chemistry, A.K. Chandra, Tata McGraw-Hill Publishing Company, 4th Edn.,1994.
2. Fundamentals of Quantum Chemistry, Anandaraman, MacMillan, India,2001
3. Grouptheoryand itsapplicationsin Chemistry, A.Salahuddin , KunjuandKrishnan, Eastern Economy Edition, 2nd edition, PHI Learning Publishers,2015.
4. P.K. Bhattacharya, Group Theory and Its Chemical Applications, Himalayan Publishing House, 1986.
5. V. Ramakrishnan and M.S. Gopinathan, Group Theory in Chemistry, VishalPublications, 1998.

Reference Books:

1. Quantum Chemistry, R.K. Prasad, Wiley Eastern, New Delhi,1992.
 2. Introductory Quantum Mechanics, Y.R. Waghmare, Eurasia Publishing House, NewDelhi, 1989.
 3. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley-Interscience Publications, 2006.
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M.Sc. CHEMISTRY (II SEMESTER)

18CHEP0210

Inorganic Chemistry Practical-I

(2credit)

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. Tetraamminecopper(II) Sulphate
- c. Hexaamminechromium(III) Nitrate
- d. Hexaamminechromium(III) Chloride
- e. Tris(ethylenediamine)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

Text Book:

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

Reference Book

1. Experimental Inorganic Chemistry, W.G. Palmer, Cambridge University Press, Cambridge, 1965.
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M.Sc. CHEMISTRY (II SEMESTER)

18CHEP0211

Physical Chemistry Practical–II

(2credit)

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 chemisorption 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. Study on saponification of ethyl acetate by conductometry and determination of the order of reaction.
 3. Determination of the rate constant and order of reaction for the reaction between potassium persulphate and potassium iodide.
 4. Study of the kinetics of the reactions between iodine in acidic medium by half-life method and determination of order with respect to iodine and acetone.
 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. To determine the concentration of sugar in a solution refractometrically.
 9. Determination of composition of a mixture of liquids refractometrically.
 10. Estimation of concentration of a mixture by colorimetric method.
 11. Determination of activation energy for the acid catalyzed hydrolysis of methylacetate.
 12. Determination of hydrolysis constant of aniline hydrochloride by conductometry.

Text Books:

1. Senior Practical Physical Chemistry, D.D. Khosala, A. Khosala, V.C. Gard, R.Chand & Co., New Delhi, 1975.
2. Practical Physical Chemistry B. Viswanathan and P.S. Raghavan, Viva Books Pvt. Ltd., New Delhi, 2008.

Reference Books

1. Experimental Physical Chemistry Ed, by E. Daniels, International Student Edn., McGraw Hill, 1970.
 2. Experimental Physical Chemistry, G. Peter Mathews, Oxford Science Publications, 1985.
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M.Sc. CHEMISTRY (III SEMESTER)

18CHEP0312

Inorganic Chemistry– III

(3 credit)

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 pentacarbonyl 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. Rings: Synthesis and reactions of borazines, phosphazenes, phosphazene polymers - Structures and bonding of phosphazene. Cages: Phosphorus, phosphorus trioxide and pentoxide - Boron compounds - Higher boron hydride classification and electron counting. Clusters: Dinuclear, tetranuclear and hexanuclear cluster - Polyatomic zintl anions and cations - Chevrel phases.

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 - Carbonic

anhydrase and Carboxypeptidase, Oxygen transport, Iron-sulphur proteins-rubredoxin, ferriedoxin, nitrogen fixation- anti cancer activity of platinum complexes.

Text Books:

1. Inorganic Chemistry, J.E. Huheey, E.A. Keither and R.L. Keiter, Harper Collins College Publisher, 4thEdn., New York, 1993.
2. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and C.H. Langford, ELBS, Oxford University Press, 2000.
3. Principles of Organometallic Chemistry, P.Powell, Chapman and Hall, London,1988.
4. Lehninger Principles of Biochemistry, D. L. Nelson, M. M. Cox, Freeman & Company, New York, 2005.

Reference Books:

1. Inorganic Chemistry, G.L. Miessler and D.A.Tarr, Pearson, Prentice Publishers, Delhi, 2009.
 2. Inorganic Chemistry, B.Douglas, D.H. McDaniel and Concepts and Models of J.J. Alexander, John Wiley and Sons, New Delhi, 2001.
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M.Sc. CHEMISTRY (III SEMESTER)

18CHEP0313

Organic Chemistry–III

(3credit)

Objectives: The objective of the course is to understand conformational analysis of acyclic and cyclic organic compounds, to know the basic principles involved in mass spectrometry and also combined spectroscopy problems involving simple organic molecules, to understand organic chemical reactions involving structural changes, to know the mechanism of action, synthetic utility of some important organic reactions and reagents and to understand the chemistry of selected alkaloids and heterocyclics.

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

- *Predict and analyze the conformations of acyclic and cyclic organic compounds.*
- *Interpret mass spectral data Analyze and identify simple organic molecules by using UV, IR, Mass, ¹H NMR and ¹³C NMR data.*
- *Assess the mechanism and synthetic uses of selected reagents and reactions.*
- *Elucidate the structure and plan for the synthesis of selected alkaloids.*

Unit I – Conformational Analysis

Conformational Analysis of acyclic system: Conformations of ethane and butane, conformation of halogenoalkanes, conformation of diastereoisomers- 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-Skita rule- conformations of cis and trans-decalins. Conformations of perhydroanthracene and perhydrophenanthracene - conformationally rigid and mobile diastereomer, quantitative correlation between conformation and reactivity, Winstein- Elie equation, Curtin- Hammett principle, Steric assisted and steric hindered reactions.

Unit II – 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 III – Molecular Rearrangements

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

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

Oxidation: Mechanism and applications of reaction involving oxidation with CrO₃, OsO₄, SeO₂, NaIO₄, mCPBA and Swern oxidation.

Reduction: Mechanism and applications of reaction involving reduction with NaBH₄, LiAlH₄, DIBAL-H, Bu₃SnH. Name Reactions: Robinson annulations, Suzuki Coupling, Wittig reaction, Stark enamine synthesis and Shapiro reaction.

Unit V – Alkaloids

Structural elucidation and synthesis of following alkaloids: piperine – nicotine –quinine - atropine and morphine.

Text Books:

1. A Guide Book to Mechanism in Organic Chemistry, P. Sykes, Orient Longman, 6thEdn., 1988.
2. Spectrometric identification of organic compounds, R.M. Silverstein, F.X. Webster, D.J. Kiemle, 7thEdn., John Wiley & Sons, New Delhi, 2006.
3. Organic Spectroscopy, W. Kemp, ELBS, 2ndEdn., 1991.
4. Organic Chemistry, I.L. Finar, Vol.2 ELBS, 5thEdn., 1974.
5. Organic Reaction Mechanisms, Raj K. Bansal. New Age International Publishers, 4thEdn., New Delhi, 2012.
6. Organic Reactions and their Mechanisms, P.S. Kalsi, New Age International Publishers, New Delhi, 1996.
7. Molecular Reactions and Photochemistry, C.H. DePuy and O.L. Chapman, Prentice-Hall, New Delhi, 1987.
8. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Publishers, 6thEdn., New Delhi, 2005.
9. Stereochemistry of Organic Compounds: Principles and Applications, D. Nasipuri, New Age International Publishers, 2ndEdn., New Delhi, 2005.
10. Moderns Methods of Organic Synthesis, W. Carruthers, and I. Coldham, Cambridge University Press, UK, 4thEdn., 2004.

Reference Books

1. Advanced Organic Chemistry. Part-A. Structure and Mechanisms, F. Carey, R. Sundberg, 4th Ed., Kluwer Publishers, 2000.
 2. March's Advanced Organic Chemistry, Michael B. Smith, J. March John Wiley & Sons, 6thEdn., 2007.
 3. Organic Chemistry, J. Clayden, N. Greeves, P. Wothers, Oxford University Press, 2001.
 4. Organic Chemistry, J. Mc. Murry, Brooks/Cole publisher, 5thEdn., 2000.
 5. Organic Synthesis, M. B. Smith, Academic Press, Elsevier, 3rdEdn., 2010.
 6. Stereochemistry of Carbon Compounds, E.L. Eliel, McGraw Hill Book Company, New York, 1975.
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M.Sc. CHEMISTRY (III SEMESTER)

18CHEP0314

Physical Chemistry–III

(3credit)

Objectives: The objective of the course is to understand the theories of microwave, 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 pathways in photochemical 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 of polyatomic molecules-Linear symmetric top and asymmetric top molecules, chemical analysis by microwave spectroscopy. Diatomic vibrating rotator, vibrations, rotational spectrum of CO, vibrations of polyatomic molecules, 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-chemical shift, quadrupole effect, magnetic field effect.

Unit III - Molecular Spectroscopy III

Nuclear magnetic spectroscopy-nuclear spin, factors influencing chemical shift, deshielding, spin-spin interactions. Introduction to ^{13}C NMR-chemical shift-charge density calculation-broad band decoupling-off resonance decoupling and gated decoupling.

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, micro emulsions. Principle, instrumentation and applications of ESCA, SERS and Auger spectroscopy.

Text Books:

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

Reference Books

1. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1962.
 2. Principles of colloids and surface chemistry, P. C. Heimenz, R. Rajagopalan, Taylor & Francis, 3rdEdn., 1997.
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M.Sc. CHEMISTRY (III SEMESTER)

18CHEP0315

Inorganic Chemistry Practical-II

(2credit)

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 and nickel
 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.

Text Book:

1. Vogel's Text book of quantitative Chemical analysis, G.H. Jaffery, J. Bassett, J. Mendham and R.C. Deeny. ELBS, 1997.

Reference Book:

1. Analytical Chemistry in Metallurgy, V.I. Posypaiko and N.A. Vasiua, Mir Publisher, Moscow, 1984.
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M.Sc. CHEMISTRY (III SEMESTER)

18CHEP0316

Organic Chemistry Practical-II

(2credit)

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.
5. Resolution of racemic compounds.
6. Green synthesis and multi-component synthesis of selected compounds.

Text Books:

1. Laboratory Manual of Organic Chemistry, Dey and Sitaraman, Allied Publishers, 1992.
2. Organic Chemistry Lab Manual, N. S. Gnanaprakasam, G. Ramamurthy, S. Viswanathan Printers and Publishers Pvt. Ltd., 2015.

Reference Books:

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, 5th Edn., England, 1989.
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M.Sc. CHEMISTRY (III SEMESTER)

18CHEP0317

MiniProject

(1credit)

The candidate will be required to submit a report based on the literature survey and pre-liminary 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)

18CHEP0418

Inorganic Chemistry-IV

(4Credit)

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-block elements.

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 PCl_5 - 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^* , $\pi - \pi^*$ and $\pi - d$ energy states. Photochemical reactions of metal complexes – substitution- Admson's rules- rearrangement– isomerisation– racemisation– aquation and anation – redox reactions. Ruthenium polypyridyls – excited state properties – electron transfer and energy transfer quenching reactions – importance of solar energy conversion and storage – cleavage of water using Ru(bpy)₃²⁺, Cadmium sulphide colloidal particles and titanium dioxide semiconductor – [Ru(edta)H₂O] catalyzed ammoniaproducton.

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.

Text Books:

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, 4th Edn, 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.

Reference Books:

1. Radiochemistry and Nuclear Chemistry, G. Choppin, J-O. Liljenzin, J. Rydberg, Butterworth-Heinemann Publishers, 3rd Edn., 2002.
 2. Organic and Inorganic Photochemistry in Molecular and Supramolecular Chemistry, Vol. II, Eds. V. Ramamurthy, K. S. Schanze, Marcel Dekker Inc., New York, 1998.
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M.Sc. CHEMISTRY (IV SEMESTER)

18CHEP 0419

Organic Chemistry-IV

(4credit)

Objectives: The objective of the course is to enable students to know various strategies used in retro synthetic analysis, chemistry of various organic reagents and also to know the chemistry of selected steroids, hormones and bioorganics.

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

- Describe the important concepts of the organic chemistry for the synthesis of new molecule, introduction of different functional group.
- Assess the synthetic uses of selected organic reagents.
- 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, insulin and oxytocin.
- Explain the chemistry involved in vitamins B₁, B₆ and C, proteins, structure and coupling reagents, nucleic acids and structure, synthesis of antibiotics.

Unit I - 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 - umpolung reactions - typical examples of one group C-X and two group C-X disconnections – two group disconnections – 1,2-difunctionalised compounds – 1,3- difunctionalised compound and □□□-unsaturated carbonyl compounds – 1,4-difunctionalised compounds – Diels – Alder reactions and Michael additions.

Unit II - Organic Reagents-I

Study of synthetic applications of the following reagents - LDA, LiHMDS, DMAP, Na-Liq.NH₃, DDQ, Pd(PPh₃)₄, Simmon-Smith Reagent, Gilman's Reagent, Woodward & Prevost Hydroxylation and Peterson's Synthesis.

Unit III - Organic Reagents-II

Study of synthetic applications of the following reagents – n-BuLi, Et₂Zn, CBS-catalyst, EDCI, DCC, HATU, HOBT, CAN, TEMPO and IBX.

Unit III-Protection and Deprotection Chemistry in Organic Synthesis and Green Chemistry

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 of 1,2 and 1,3-Diols-methylene dioxyderivative: Methoxymethylene acetal, ethylene acetal, 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.

UnitV - Steroids and proteins

Synthesis of Cholesterol– Conversions of cholesterol to Androsterone, Testosterone, Progesterone.

Proteins: Structure of Proteins-End group analysis-Primary, Secondary, Tertiary and Quaternary Structure of protein. Chemistry and structure of oxytocin.

Text Books:

1. Organic Synthesis: The Disconnection Approach, Stuart Warren, Paul Wyatt, Wiley, 2ndEdn.,2008.
2. Advanced Organic Chemistry Part-A, F.A. Carey and R.J. Sundberg, Springer, 5thEdn., 2007.
3. Advanced Organic Chemistry Part-B, F.A. Carey and R.J. Sundberg, Springer, 5thEdn., 2007.
4. Moderns Methods of Organic Synthesis, W. Carruthers, and I. Coldham, Cambridge University Press, UK, 4thEdn., 2004.
5. Protective Groups in Organic Synthesis: Theodora W. Greene and Peter G. M. Wuts, John Wiley & Sons, Inc.,3rdEdn., 1999.
6. Organic Synthesis Special Techniques, V.K. Ahluwalia, Renu Aggarwal, Narosa publishing House, 2004.
7. Recent Developments of Peptide Coupling reagents in Organic Synthesis: So-Yeop Han and Young-Ah Kim, Tetrahedron 2004, 60, 2447-2467.
8. Organic Chemistry, I.L. Finar, Vol.2 ELBS, 5thEdn.,1974.

Reference Books

1. March's Advanced Organic Chemistry, Michael B. Smith, J. March John Wiley & Sons, 6thEdn.,2007.
2. Advanced Organic Chemistry Reactions, Mechanisms and Structure, M. B. Smith and J. March, Wiley, 6th Edn., 2007.
3. Organic Chemistry, J. Mc. Murry, Brooks/Cole publisher, 5thEdn., 2000.
4. Organic Synthesis, M. B. Smith, Academic Press, Elsevier, 3rdEdn., 2010.

M.Sc. CHEMISTRY (IV SEMESTER)

18CHEP0420

Physical Chemistry-IV

(4credit)

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.

Unit II - Statistical Thermodynamics II

Bose-Einstein statistics-Fermi-Dirac statistics-comparison of the three statistics- applications-use of partition functions for obtaining thermodynamic functions-Gibbs free energy-entropy and probability-Boltzmann-Planck's equation-statistical approach to third law of thermodynamics and exception of this law-molar partition function-specific heat of solids-Einstein theory of specific heat-Debye theory.

Unit III - Chemical Kinetics I

Theories of reaction rates-absolute reaction rate theory-thermodynamic formulation of ARR theory-Lindeman's theory of unimolecular reactions, Marcus theory of electron transfer process. Derivation 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). Effect of temperature, relative permittivity, ionic strength and solvent on reaction rates.

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. Experimental methods for the study of fast reactions-flow method-relaxation methods-flash methods-nuclear magnetic resonance method.

Text Books:

1. Physical Chemistry, P. W. Atkins, Oxford University Press, 1998.
2. Chemical Kinetics and Dynamics, J.J. Steinfeld, J.S. Francisco and W.L. Hase, 2nd Edn., Prentice Hall, New Jersey, 1999.

Reference Books:

1. Physical Chemistry, R. Stephen Berry, S.J. Rice, and J. Ross, 2nd Edn., Oxford University press, New York, 2000.
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M.Sc. CHEMISTRY (IV SEMESTER)

18CHEP0421

DISSERTATION

(4Credit)

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.

M.Sc. CHEMISTRY (III SEMESTER)

Major Electives

18CHEP03E1

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 polymerchemistry.*
- *Explain the basic concepts of polymer synthetic techniques.*
- *Analyze the basic reactions in polymerchemistry.*
- *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, Stereo regular polymerization, Condensation polymerization – Mechanism and Kinetics of polymerization – degree of polymerization – kinetic chain length – factors affecting chain polymerization- inhibition and retardation – Carother's equation.

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 – management of plastics in the environment.

The concept of number average and weight averages. Molecular weight methods - Molecular weight distribution, separation of polymers – precipitation and isolation by gel permeation chromatography - 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 T_m – melting points of homogeneous series – effect of chain flexibility and heat of fusion. The glass transition temperature, T_g -relationship between T_m and T_g , effects of molecular weight,

chemical structure, property requirements and polymer utilization. Fabrications of polymers – Moulding, casting and spinning polymers.

Unit V – Chemistry of Commercial Polymers and Polymer Additives

Organic polymers polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins. Dendrimers – Types and applications. Inorganic polymers – silicon polymers, glass, poly (organophosphazenes) polymers, Basic concept of conducting polymers, liquid crystal polymer, biopolymer and biomedical polymer. Polymer additives: Fillers, plasticizers, colourants, auto oxidants, fire retardants and thermal stabilizers – polymer blends and composites.

Text Books:

1. Text book of polymer science, F.W. Billmeyer Jr. 3rdEdn., Wiley, India 2007.
2. Polymer science, V.R. Gowarikar, N.V. Viswanathan, New age international, 2003.
3. Polymer science and technology of plastics and rubbers, P. Ghosh, Tata McGraw-Hill, New delhi, 1998.
4. Introductory polymer chemistry, G.S. Misra, Wiley eastern Ltd., 1993.

References

1. Principles of polymerization, George Odian, 4thEdn., John wiley and sons, 2007.
 2. Polymer science and technology, Goel R. Fried, Prentice – Hall of India, New delhi, 2000.
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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 thermodynamics. 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 ρ -values. Reaction constant. Deviations from Hammett equation. Dual-Parameter correlations, inductive substituent constant. The Taft model, S_1 and S_R 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.

Text Books:

1. Kinetics and Mechanisms of Chemical Transformations, J. Rajaram, J.C. Kuriacose, MacMillan India Ltd., 1998.
2. Physical Organic Chemistry, N.S. Isaacs, Longman, 1998.
3. An Introduction to Physical Organic Chemistry, E.M. Kosower, John Wiley & Sons, New York, 1968.

Reference Books:

1. Physical Organic Chemistry, C.D. Ritchie, Marcel Dekker Inc., New York, 1990.
 2. Correlation Analysis of Organic Reactivity, J. Shorter, Research Studies Press, Chichester, 1998.
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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

Physicochemical properties in relation to biological action - influence of route of administration. Biotransformation-absorption from stomach -absorption from intestines -sites of loss -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-Cephalosporin and Tetracycline. Polyene antifungal antibiotics-nystatin, fusidic 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. Antipyretic analgesics - salicylic acid, pyrazole and para amino phenol derivatives. Sedatives:- Barbiturates, Benzodiazepines.

Unit IV - Cardio Vascular and anti-tubercular drugs

Cardio Vascular Drugs -classification, cardiac glycosides, anti-hypertensive and hypotensive agents -mode of action -anti-arrhythmic 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.

Text Books:

1. Text book of organic, Medicinal and Pharmaceutical Chemistry, O. Wilson, O. Giswold and F. George, Lippincott Company, Philadelphia, 9th Edn., 1991.
2. Text book of Pharmaceutical Chemistry, Bentley and Driver

Reference:

1. Medicinal Chemistry Vol - I and II, A. Burger, Wiley Inter Science, New York, 1990.
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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 to 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 - oil spills - oil spill removal methods - disease causing agents.

Unit II - Air Pollution

Atmosphere - structure - functions and photochemical reactions - sources of air pollution - Natural and manmade - classification and effects of air pollutants - CO, CO₂, SO₂, SO₃, NO and NO₂ - 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 hormones, 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 SO₂ by spectrophotometer.

Text Books:

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

References:

1. Environmental Chemistry: Fundamentals, J. G. Ibanez, M. Hernandez-Esparza, C. Doria-Serrano, A. Fregoso-Infante, M. Mohan Singh, Springer Publishers, 2007.
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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 cations, anions 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 $^1\text{H-NMR}$ 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 ball dimer.

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 $\text{OH}\dots\text{O}$, $\text{NH}\dots\text{O}$, $\text{OH}\dots\text{N}$ and $\text{NH}\dots\text{N}$ 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-chain supramolecular polymers, examples of stimuli responsive supramolecular polymers and self-healing polymers.

Text Books:

1. Supramolecular Chemistry - A Concise Introduction, J. W. Steed and J. L. Atwood, John Wiley, 2000.
2. Supramolecular Chemistry of Anions, Ed: Antonio Bianchi, Kristin Bowman James and Enrique Garcia-España, Wiley-VCH 1997.
3. Anion Receptor Chemistry. Ed: Jonathan L. Sessler, Philip A. Gale and Won-Seob Cho, RSC Publishing, 2006.
4. Analytical Methods in Supramolecular Chemistry. Ed: Christoph Schalley, Wiley-VCH

Verlag GmbH & Co.,2007.

5. Crystal engineering using multiple hydrogen bonds, In Structure and Bonding, Ed: Andrew D. Burrows, Vol. 108, 55-96, 2004.

Reference Books:

1. Modern Supramolecular Chemistry-Strategies for Macrocyclic Synthesis, Ed: François Diederich, Peter J. Stang and Rik R. Tykwinski, Wiley-VCH Verlag GmbH & Co.,2008.
 2. Supramolecular Chemistry: From Biological Inspiration to Biomedical Applications, Peter. J. Cragg, Springer Publishers, 2010.
 3. Organic Nanostructures. Ed: Jerry L. Atwood and Jonathan W. Steed, Wiley-VCH Verlag GmbH & Co.,2008.
 4. Supramolecular polymers. Ed: Alberto Ciferri, 2ndEdn., CRC Press,2005.
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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 groups and functional group interconversion by substitution reactions.

Unit I –Asymmetric Synthesis

Basic principles of Asymmetric synthesis – Definition - Stereospecific, Stereoselective – enantioselective 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, trans-1,2-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 $\text{BH}_3\text{:THF}$, Catecholborane, $\text{Na}(\text{CN})\text{BH}_3$, Raney nickel, Zn in acidic media, Lindlar catalyst, $\text{Al}(\text{O}i\text{Pr})_3$, Rosenmund Reduction.

Unit III - Name reactions

Reaction and Mechanism of following name reaction: Arndt-Eistert Synthesis, 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 Robinson annulations.

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 sitagliptin, Linagliptin, Saxagliptin. Proton pump Inhibitors-Synthesis of omeprazole, lansoprazole, pantoprazole. Sulphadruugs –Synthesis of sulphathiazole, sulphamerazine, sulphaguanidine.

Text Books:

1. Advanced Organic Chemistry Part A, F. A. Carey and R. J. Sundberg, Springer, 5thEdn., 2007.
2. Advanced Organic Chemistry Part B, F. A. Carey and R. J. Sundberg, Springer, 5thEdn., 2007.
3. Organic Chemistry, I.L. Finar, Vol.2 ELBS, 5thEdn.,1974.
4. A Guide Book to Mechanism in Organic Chemistry, P. Sykes, Orient Longman, 6thEdn., 1988.
5. Moderns Methods of Organic Synthesis, Carruthers, W. and Coldham, I, Cambridge University Press, UK, 4thEdn.,2004.
6. Advanced Organic Chemistry Reactions, Mechanisms and Structure, M. B. Smith and J. March, Wiley, 6thEdn., 2007.

References

1. Stereochemistry of Organic Compounds, E.L. Eliel, Samuel H. Wilen, Wiley – India Edition 2008.
2. Advanced Organic Chemistry Reactions, Mechanisms and Structure, M. B. Smith and J. March, Wiley, 6thEdn., 2007.
3. Mathad, V. T.; Govindan, S.; Kolla, N. K.; Maddipatla, M.; Sajja, E.; Sundaram, V.; *Organic Process Research & Development* **2004**, *8*, 266-270.
4. 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.
5. Desai, A. A. *Angew. Chem. Int. Ed.* **2011**, *50*, 1974 – 1976.
6. Organic Chemistry, J. Clayden, N. Greeves, P. Wothers, Oxford University Press, 2001.
7. Organic Chemistry, J. Mc. Murry, Brooks/Cole publisher, 5thEdn., 2000.
8. Organic Synthesis, M. B. Smith, Academic Press, Elsevier, 3rdEdn., 2010.

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 – Knoevenagel condensations – Wittig reactions – Phase transfer catalyst - Synthesis – applications of Quaternary ammonium salts.

Unit-IV: Ultrasound Assisted organic synthesis (UAOS)

Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizzaro 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, Benzoylation 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-villiger-oxidation).

Text Books:

1. New Trends in Green Chemistry, V.K. Ahluwalia & M.R. Kidwai, Anamalaya Publishers (2005).
2. Green Chemistry – Environmentally benign reactions, V. K. Ahluwalia, Ane Books India (Publisher), 2006.
3. Green Chemistry-Theory and Practical, Anastas, P.T. & Warner, J.K. Oxford University Press(1998).
4. Green Chemistry – Environment friendly alternatives- Ed. Rashmi Sanghi & M. M. Srivastava, Narora Publishing House, 2003.
5. Organic Reactions in Water: Principles, Strategies and Applications-U. M. Lindstrom; Blackwell Publishing Ltd, 2007.

Reference Books:

1. Green Chemistry-An Introductory Text; Mike Lancater; RSC publishers2011.
 2. Green Chemistry – Designing Chemistry for the Environment – edited by Paul T. Anastas& Tracy C. Williamson. Second Edition,(1998).
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Non-Major Electives

18CHEP02N1

ELEMENTSOFBIOCHEMISTRY

(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 enzyme inhibitors.

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, encapsulation), applications of immobilized enzyme systems, effect of immobilization on K_m , 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.

Text Books:

1. Lehninger Principles of Biochemistry, D. L. Nelson, M. M. Cox, Freeman & Company, New York, 2005.
2. Elements of Biotechnology, P.K. Gupta, Rastogi Publications, 1st Edn., 1994.
3. Biochemistry, S.C. Rastogi, Tata Mc.Graw Hill, 1st Edn., 1993.

Reference Books:

1. Biotechnology, M.D. Travan, S. Boffev, Tata McGraw Hill, 1stEdn., 1987.
2. Biotechnology, K. Trehan, Wiley Eastern Ltd., 1stEdn., 1990.
3. Outlines of Biochemistry, E.E. Conn, P.K. Stumpf, Wiley Eastern Ltd., 4thEdn., 1976.

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 methods and what techniques should be used for the analysis to solve a particular problem.*
- *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.

Text Books:

1. Principles of Instrumental methods of analysis, Skoog and West, Saunders College Publications, 1992.
2. Instrumental methods of chemical analysis, B.K. Sharma, Goel publishing House, 19th Edn., 2000.
3. Electrochemical Methods, Fundamentals and Applications, A.J. Bard and L.R. Faulkner, John Wiley & Sons, 2nd Edn., 2001.

Reference Books

1. Instrumental methods of analysis, H.W. Willard, L.I. Merrit, J.J.A. Dean and F.A. Settle, CBS publishers, 1983.
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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, CO₂, SO₂, SO₃, NO and NO₂ – 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 CO₂ by spectrometry. Treatment of water for domestic and industrial purpose – primary, secondary and tertiary treatment methods.

Text Books:

1. Chemical and Biological Methods for Water Pollution Studies, R.K. Trivedy and P.K. Goel, Environmental Publications, 1986.
2. Engineering Chemistry, P.C. Jain and Monica Jain, Dhanpat Rai & Sons, 1993.
3. Text book of Environmental Chemistry, C.D. Tyagi and M. Mehra, Anmol Publishers, 1996.
2. Fundamentals of Environmental Pollution, K. Kannan, S. Chand & Co., 1997.
3. Environmental Chemistry, A.K. De, Wiley Eastern Ltd, 3rd Edn., 1994.
4. Environmental Chemistry, B.K. Sharma, Goel Publishers, 2001.
5. Environmental Chemistry, M.S. Sethi, Sri Sai Printographers, 1994.

References:

1. Water Quality and Defluoridation Techniques, Rajiv Gandhi National Drinking Water Mission Publication, 1994.
2. Environmental Chemistry: Fundamentals, J. G. Ibanez, M. Hernandez-Esparza, C. Doria-Serrano, A. Fregoso-Infante, M. Mohan Singh, Springer Publishers, 2007.

Modular Courses

18CHEP03M1

ADVANCEDFUNCTIONALMATERIALS

(2credits)

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 PAMAM, 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.*
- *Describe the principles underlying the high temperature superconductors and applications of oxide materials.*
- *Identify the structure and importance of various biodegradable polymers, supramolecular polymers and self-healing polymers.*

Unit I - Molecular-Level Devices and Machines

Molecular machines: Pseudorotaxanes, rotaxanes and catenanes – Systems featuring charge-transfer interactions – systems featuring hydrogen bonding interactions. Devices based on Electronic and Nuclear motion: Plug/socket and related systems – electrochemically controlled systems.

Unit II - Poly(amidoamine) Dendrimer-Based Multifunctional Nanoparticles

PAMAM Dendrimers: Structure and biological properties – Synthesis and characterization, PAMAM dendrimers as a vehicle for molecular delivery into cells – PAMAM dendrimers as MRI contrast agents.

Unit III - Advanced functional oxide materials and their applications

High temperature superconductors: Cuprate Materials, Electrical and Magnetic properties - Magnetic oxide materials: Ferromagnetic oxide materials, Ferrites materials - Multiferroic Materials : Origin of magnetic ordering in the oxide materials.

Unit IV - Biodegradable Polymers

Biodegradable polymers - poly -caprolactone- modified poly -caprolactone copolymer with ester, amide and urethane linkages, polyglycolate, poly mandelic 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.

Text Books:

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. High Temperature Superconductivity, J. W. Lynn, Springer-Verlag, 1990.
4. 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.

References

1. Polymers and Ecological problems, Ed., J. Guillet, Plenum Press, New York, 1973.
 2. Polymer Degradation – Principles and Practical Applications, W. Schnabel, Hanser International, 1981.
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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 cancerous cells.

Unit V - Nanotechnology in Nature

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

Text Books:

1. Nano: The Essentials: Understanding Nanoscience and Nanotechnology, T. Pradeep, McGraw-Hill Professional Publishing, 2008.

Reference Book:

1. Introduction to Nanoscience, J. Dutta, H.F. Tibbals and G.L. Hornyak, CRC press, Boca Raton, 2008.
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18CHEP04M1 MOLECULAR ELECTRONICS AND ORGANICPHOTOVOLTAICS
(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 moleculelectronics.*
- *Plan for the fabrication of moleculedevices.*
- *Identify the methods of probing individualmolecules.*
- *Explain the organicphotovoltaics*

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.

Text Books:

1. Introducing Molecular Electronics by Cuniberti, Gianaurelio, Fagas, Giorgos, Richter, Klaus (Eds.), 2005, Springer Publishing, Chennai.
2. Molecular Electronics - Commercial Insights, Chemistry, Devices, Architectureand Programming by James M Tour,2003, First Edition, World Scientific Publishing Company,Singapore.

References:

1. Molecular Electronics - An Introduction to Theory and Experiment by Juan Carlos Cuevas and ElkeScheer, 2010, First Edition, World Scientific Publishing Company, Singapore.
2. Third Generation Photovoltaics Advanced Solar Energy Conversion, Martin A. Green, Springer, 1st Ed.2003.

18CHEP04M2 WATER QUALITY MONITORING, MANAGEMENT AND TREATMENT (2 credits)

Objectives: The objective of the course is to give 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-fluoride - iron - arsenic - mercury/Algal analysis plankton analysis - biomass and chlorophyll estimation - microbial examination - standard plate count - MPN of coliforms - estimation of MPN - bioassay - requirements of bioassay.

Unit II - Ground water and surface water pollution and control measures

Surface water 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. Demineralisation of water for industrial purposes - boiler problems - scale and sludge formation - prevention of scale formation - internal and external treatment - lime soda - 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 industrial effluents.

Unit V - Water Management

Water resources management - rain water harvesting methods - percolation ponds - check dams - 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.

Text Books:

4. Chemical and Biological Methods for Water Pollution Studies, R.K. Trivedy and P.K. Goel, Environmental Publications, 1986.
5. Engineering Chemistry, P.C. Jain and Monica Jain, Dhanpat Rai & Sons, 1993.
6. Text book of Environmental Chemistry, C.D. Tyagi and M.Mehra, Anmol Publishers, 1996.
6. Fundamentals of Environmental Pollution, K. Kannan, S. Chand & Co., 1997.
7. Environmental Chemistry, A.K. De, Wiley Eastern Ltd, 3rd Edn., 1994.
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9. Environmental Chemistry, M.S. Sethi, Sri Sai Printographers, 1994.

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3. Water Quality and Defluoridation Techniques, Rajiv Gandhi National Drinking Water Mission Publication, 1994.
 4. Environmental Chemistry: Fundamentals, J. G. Ibanez, M. Hernandez-Esparza, C. Doria-Serrano, A. Fregoso-Infante, M. Mohan Singh, Springer Publishers, 2007.
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