



RAYALASEEMA UNIVERSITY

M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)

I Semester Syllabus under CBCS

(Effective from the academic year 2015-2016)

S.No	Paper Number	Title of Paper	No. Of Credits	University Exam Duration(Hrs)	Total Marks	
					IA	SEE
1	CHEM-OC/NP101: Paper I	Inorganic Chemistry -1 (Common to OC & NP)	4	3	30	70
2	CHEM-OC/NP102: Paper II	Organic Chemistry-I (Common to OC & NP)	4	3	30	70
3	CHEM-OC/NP103: Paper III	Physical Chemistry – I (Common to OC & NP)	4	3	30	70
4	CHEM-OC/NP104: Paper IV	Chemical Group Theory, Spectroscopy & Errors in Chemical Analysis (Common to OC & NP)	4	3	30	70

IA : Internal Assessment = IAE (25) + SS (5)

SEE : Semester End Examination

IAE : Internal Assessment Examination

SS : Student Seminar

RAYALASEEMA UNIVERSITY: KURNOOL
M Sc., ORGANIC CHEMISTRY (OC)/NATURAL PRODUCTS (NP)
I SEMESTER SYLLABUS under CBCS
(EFFECTIVE FROM THE ACADEMIC YEAR 2015-2016)
CHEM-OC/NP: 101: PAPER-I INORGANIC CHEMISTRY –I

UNIT-I : Metal Ligand Bonding and Magnetic Behaviour of Complexes
UNIT-II : Metal Ligand equilibria in solution and theory of HSAB
UNIT-III : Metal carbonyl and Nitrosyl Complexes
UNIT-IV: Polyacids and organometallic chemistry

Learning Objectives

- To discuss basics of coordination chemistry
- To understand the applications of organo metallic compounds
- To discuss polyacid and isopolyacids and understand the theories

UNIT-I: Metal – Ligand Bonding and Magnetic Behaviour of Complexes 15 Hours (1 Credit)

(i)Metal –Ligand Bonding: Crystal Field Theory (CFT) for bonding in transition metal complexes, crystal field splitting of d – orbitals in octahedral, tetrahedral, tetragonal and square planar fields. Crystal Field Stabilization Energy (CFSE) and its calculation in six and four coordinated complexes, Spectrochemical series with reference to ligands and metal ions. Factors affecting the magnitude of Δ_o in octahedral complexes, Jahn- Teller effect and its consequences. Shortcomings of CFT; Covalency: Evidence for covalency, Nephelauxetic effect; Molecular orbital theory: Concept of Ligand Group Orbitals (LGOs), MO diagrams for octahedral, tetrahedral and square planar complexes, MO treatment of π -Bonds.

(ii)Magnetic Behaviour of Complexes: Types of magnetic behavior, Temperature independent paramagnetism. Magnetic susceptibility and its determination by Gouy's and Faraday's methods. Calculation of Magnetic moment from magnetic susceptibility, spin-only formula, orbital contribution to magnetic moment (Oh and Td Complexes)

UNIT-II: Metal –Ligand equilibria in solution and theory of HSAB 15 Hours (1 Credit)

(i)Metal-ligand equilibria in solution

Stepwise and overall formation constants and their interrelationship, Trends in stepwise formation constants, factors affecting the stability of metal complexes, Chelate effect, Determination of binary formation constants by pH-metry and spectrophotometric methods.

(ii) Theory of HSAB

Hard and soft acids and bases, Classification, Acid-Base strength and hardness, Symbiosis, Electronegativity and hardness, Application of HSAB: Biological functions and toxicology of metals, and medicinal applications.

UNIT-III: Metal carbonyl and Nitrosyl Complexes

Nature of π bonding, classification of π ligands, effect of π bonding on the ligand field splitting energy of octahedral complexes. π -bonding and spectrochemical series, π -donor ligands and π -acceptor ligands

Metal carbonyls: Synthesis of metal carbonyls, structures of metal carbonyls of the types $M(\text{CO})_n$ ($M=\text{Cr, Fe, Ni}$; $n=4-6$), $M_2(\text{CO})_n$ ($M=\text{Co, Fe, Mn}$; $n=8-10$), $M_3(\text{CO})_{12}$ ($M=\text{Fe, Ru and Os}$) $M_4(\text{CO})_{12}$ ($M=\text{Co, Rh, and Ir}$). IR spectra of metal carbonyls- (i) Detection of bridging CO ligand, (ii) Determination of molecular symmetry and (iii) Determination of bond angles in metal carbonyls. Synergistic effect, EAN and 18- electron rules as applied to metal carbonyls, Electron counting methods- (i) Oxidation State method and (ii) Neutral Atom method, Applications of Metal Carbonyls

Metal Nitrosyls : Synthesis of metal nitrosyls, Bonding, Electron donation by nitric oxide, Principles of stoichiometry, Models for NO bonding – (i) Covalent model and (ii) Ionic models, Structures of Metal nitrosyls (1) $[\text{IrCl}(\text{PPh}_3)_2(\text{CO})(\text{NO})]^+$, (2) $[\text{RuCl}(\text{PP}_3)_2(\text{NO})_2]^+$, (3) $[(\text{Cp})\text{CrCl}(\text{NO})_2]^+$ (4) $(\text{Cp})_2\text{Cr}_2\text{Cl}(\text{NO})_4]^+$, (5) $[\text{Co}(\text{diars})_2(\text{NO})]^{2+}$ and (6) $[\text{Co}(\text{diars})_2(\text{NO})(\text{SCN})]^+$, Detection of bridging NO ligand, Stereochemical control of valency in cobalt complexes, Applications of metal nitrosyls.

UNIT-IV: Polyacids and Organometallic Chemistry 15 Hours (1 Credit)

Polyacids: Introduction to polyacids- Types of polyacids- Isopolyacids, Isopoly molybdates, Isopolytungstates, Isopolyvanadates, Structures of Polyacids $[\text{Mo}_7\text{O}_{24}]^{6-}$, $(\text{V}_{10}\text{O}_{28})^{6-}$ and $\text{W}_4\text{O}_{16}]^{8-}$, Heteropolyacids- properties of heteropolyacids and salts, structures of heteropolyacids and theories, Mialalicopause and Roscenneium theories, Pauling's theory and keggin's theory, applications of polyacids.

Organometallic Chemistry: Introduction to 18-electron rule, Classification based on hapticity and polarity of M-C bond, nomenclature of organometallic compounds, Thermal stability-

thermochromism, Preparation, properties of methyl and phenyl organo magnesium, organo boron, organoaluminium and organo silicon compounds.

Course outcome:

- Explaining basics ideas of HSAB theory
- Understanding coordination compounds, their magnetic behavior
- Determination of stability constant by spectrophotometric methods

Reference Books

1. Inorganic Chemistry by J. E. Huheey, E.A. Keiter and R.A. Keiter, 4th edition, Harper Collins, 1993.
2. Advanced Inorganic Chemistry by F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, 6th edition, Wiley Interscience N.Y, 1999.
3. Coordination Chemistry by F. Basalo and R. Johnson (WA Benjami Inc).,1964.
4. Inorganic Chemistry, Principles and Applications by I.S. Butler and I.F. Harper, Benjami Cummings, Redwood City, CA, 1989.
5. Chemistry of Complex Equilibria, M.T.Beck, Von nostrand Reinhold,London,1990.
6. Metal Complexes in aqueous solutions, A.E.Martell and R.D. Hancock, Plenum Press New York.,1996.
7. Mechanism of Inorganic Reactions by F.Basalo and R.G.Pearson, 2nd Edn.,
8. Concise Inorganic Chemistry by J. D. Lee, 4th edition, ELBS, 1994.
9. Concise Inorganic chemistry by J.D. Lee, 5th edition, Blackwell Science Ltd. 1996.
10. Inorganic Chemistry by J.E.Huheey,E.A.Keiter and R.A.Keiter, 4th edition, Addison Wesley Publishing Company,New York,2000.
11. Chemistry of Elements by N. N. Greenwood, Pergamon press.
12. Organometallic chemistry by R.C Melhotra and A.Singh.
13. Inorganic Chemistry: G.Wulfsberg (university Science Books)
14. Modern Inorganic Chemistry W.L.Jolly, 2nd Ed. (McGraw-Hill).
15. Coordination Compounds. S.F.Kettle (Springer).
16. Magnetochemistry, R.L. Carlin(Springer-Verlag NewYork)

17. Elements of magneto chemistry R.L. Dutta and A.Syamal.2nd Ed.(AffiliatedEnst-West Press pvtLtd
18. Introdaton to Ligand Fields B.N. Higgs (Krieger pub Co)

RAYALASEEMA UNIVERSITY
M Sc., ORGANIC CHEMISTRY (OC)/NATURAL PRODUCTS (NP)
I SEMESTER SYLLABUS under CBCS
(EFFECTIVE FROM THE ACADEMIC YEAR 2015-2016)
CHEM-OC/NP: 102: PAPER-II ORGANIC CHEMISTRY –I

UNIT – 1: Stereochemistry

UNIT- II : Conformational Analysis

UNIT – III:Determination of Reactions Mechanism

UNIT- IV: Reaction Mechanism

Learning Objectives

- To develop skills in writing mechanism of organic chemistry.
- To understand conformational analysis and applying it to organic compounds
- To discuss stereochemistry.

UNIT - 1: Stereochemistry 15 Hours (1 Credit)

Molecular representations of organic molecules – Wedge, Fischer, Newman and Saw-horse formulae, their description and inter-conservation. Stereoisomerism – Definition and classification.

Molecular symmetry and chirality in organic molecules: Symmetry operations, symmetry elements (C_n , C_i and S_n) – Point group classification. Chiral point groups classifications of stereoisomers based on symmetry and energy considerations – Dissymmetric and asymmetric molecules.

Molecules with a single chiral centre: Chiral manifestations (absence of reflection symmetry, exhibiting optical activity and specific rotations etc). Molecules with a tetra-co-ordinate chiral centre (quaternary ammonium salts, N-oxides, silane derivatives, phosphines and sulfones). Molecules with a tri coordinate chiral centre (tertiary amines, carbanions, phosphines and sylfoxides). Concept of dynamic enantiomerism.

UNIT—II: Conformational Analysis: 15hours (1 Credit)

Introduction to conformational isomerism and the concept of dynamic stereochemistry, Study of conformations in ethane and 1,2-disubstituted ethane derivatives like butane, dihalobutane halohydrin, ethylene glycol, butane-2,3-diol, amino alcohols and 1,1,2,2-tetrahaloethanes.

Study of conformations of cyclohexane, mono, di and cyclohexene, cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halocyclohexanones. Stereo chemistry of decalins. Factors affecting the conformational Stability and conformation equilibrium-Attractive and Repulsive interactions. Conformational effects on the stability and reactivity of diastereomers in cyclic molecules-steric and stereo electronic factors-examples.

UNIT – III: Determination Reaction Mechanism 15 Hours (1 Credit)

- A. Energy considerations: a) Kinetics b) Reactivity and rates of reactions c) Catalysis d) Competitive reactions: thermodynamic and kinetic control e) Hammett Equation f) Curtin - Hammett Principle g) Taft Equation
- B. Important Named Reactions with Mechanism: Condensation Reactions: Aldol, Benzoin, Claisen-Schmidt, Dieckmann, Doebner, Knoevenagel and Stobbe condensation.

UNIT – IV: Reaction Mechanism: 15 Hours (1 Credit)

i) Introduction of Nucleophilic Substitution Reactions- S_N^1 , S_N^2 and S_N^1 -mechanisms and stereochemistry – Factors affecting the rate of S_N^1 and S_N^2 reactions such as substrate structure, nature of leaving group, nucleophile and the solvent.

b) **Elimination reactions:** E_2 , E_1 , E_1CB mechanisms. Orientation of the double bond-regio chemistry of the elimination reactions E_2 -syn- elimination reactions, E_2 -Anti-elimination reaction pyrolytic elimination reactions

Course outcome:

- Explaining the differences between isomerism and conformational analysis
- Identifying the molecular symmetry and molecules with a single chiral center
- Determination of energy considerations of reaction mechanism
- Discussing the named reactions and their mechanism

Reference Books

1. Stereochemistry of carbon compounds by Ernest L. Eliel
2. Stereochemistry by V.M. Potapov
3. Stereochemistry of organic compounds – Principles and applications by D. Nasipuri
4. Stereochemistry, Conformation and Mechanism by P.S. Kalsi
5. The third dimension in organic Chemistry by Alan Bassindale
6. Organic Chemistry by T.J. Solmons
7. Organic Chemistry by Robert T. Morrison and Robert N. Boyd
8. A guide book to mechanism in Organic Chemistry by Peter Sykes
9. Advanced Organic Chemistry: Reactions, Mechanism & Structure by Jerry March.
10. Reactive Intermediates by Issac
11. Mechanism and structure in Organic Chemistry by S. Mukherjee
12. Name Reactions by Jie

RAYALASEEMA UNIVERSITY
M Sc., ORGANIC CHEMISTRY (OC)/NATURAL PRODUCTS (NP)
I SEMESTER SYLLABUS
(EFFECTIVE FROM THE ACADEMIC YEAR 2013-2014)
CHEM-OC/NP: 103: PAPER-III PHYSICAL CHEMISTRY –I

Learning Objectives

- To understand the basic of concepts of Physical Chemistry.
- To learn about the fundamental concepts to modern methods of Physical Chemistry
- To explore the theoretical knowledge of physical methods into hands on experience of experimental physical chemistry.

UNIT – I: Thermodynamics- I

UNIT- II: Electrochemistry- 1

UNIT- III: Quantum Chemistry – I

UNIT –IV: Chemical Kinetics - I

UNIT - I: Thermodynamics – I : 15 Hours (1 Credit)

- i) Brief review of Thermodynamic concepts – Enthalpy, entropy, free energy. Concept of Entropy – Entropy as a state function – Entropy change in reversible process and irreversible process – Temperature – Entropy diagrams – Entropy change and Phase change – Entropy of mixing – Entropy and disorder.
- ii) Free energy and Work function: Concept of free energy – work function and free energy relationships – The Gibb's Helmholtz equations – Conditions of equilibrium – Maxwell relationships.
- iii) The third law of Thermodynamics – Entropy at absolute zero, experimental determination of entropy – Entropies of gases – Tests of the third law of thermodynamics.

UNIT – II: Electrochemistry – I : 15 Hours (1 Credit)

- i) Reversible cells – Chemical cells and concentration cells – Types of reversible electrodes – Electrode potentials. Reactions in reversible cells – Nernst equation – thermodynamic and kinetic derivation – Concentration cells with and without transference. Liquid junction potential and its determination.
- ii) Potentiometric titrations – Determination of pH, Solubility product from EMF measurements.

- iii) Theory of electrolytic conductance – Debye -HuckelOnsager equation and its verification – Wein effect. Conductometric titrations, Determination of solubility of a sparingly soluble salt.

UNIT – III: Quantum Chemistry – I : 15 Hours (1 Credit)

- i) A quick review of the following: Black body radiation – Planck’s concept of quantization (derivation not required). Photoelectric effect. Hydrogen spectrum. Bohr’s theory and its failures – Wave particle duality and uncertainty principle – Significance of these microscopic entities Emergence of Quantum mechanics.
- ii) Operators: Operators algebra – Commutation of operators, linear operators. Complex functions. Hamiltian operators. Operators ∇ and ∇^2 . Eigen functions and Eigen values. Degeneracy. Linear combination of Eigen functions of an operator, well behaved functions. Normalized and orthogonal functions.
- iii) Postulates of Quantum mechanics. Physical interpretation of wave function. Observables and operators. Measurability of properties. Average value of observable. The time dependent and time independent Schrodinger equation.

UNIT – IV: Chemical Kinetics – I : 15 Hours (1 Credit)

- i) Theories of reaction rates – Collision theory, steric factor. Theory of Absolute Reaction Rates – Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of reaction rates.
- ii) Unimolecular reactions – Lindeman’s theory – Brief explanation of HKRR and Slater’s treatments. Termolecular reactions. Complex reactions – Rate expressions for opposing, parallel and consecutive reaction (all first order type).
- iii) Chain reactions: General Characteristics, Steady State treatment $H_2 - I_2$, $H_2 - Br_2$, $H_2 - Cl_2$ reactions. Comparison of hydrogen halogen reactions. Rate expressions for chain reactions.

Course Outcome:

Students can understand the both fundamental concepts and advanced aspects of physical chemistry. It can provide a path to learn about the physical chemistry concepts of

Thermodynamics, Electrochemistry, Quantum Chemistry, Chemical Kinetics through the experiments which in turn make a platform towards research.

References:

1. Thermodynamics for Chemists by S. Glasstone.
2. Atkin's Physical Chemistry by Peter Atkins and Julio de paula.
3. Introduction to Electrochemistry by S. Glasstone.
4. Quantum Chemistry by Ira N. Levine.
5. Introduction to Quantum Chemistry by A.K. Chanda.
6. Chemical Kinetics by K.J. Laidler.
7. Atomic Structure and chemical bond by Manas Chandra.

RAYALASEEMA UNIVERSITY
M Sc., ORGANIC CHEMISTRY (OC)/NATURAL PRODUCTS (NP)
I SEMESTER SYLLABUS under CBCS
(EFFECTIVE FROM THE ACADEMIC YEAR 2015-2016)
CHEM-OC/NP: 104: PAPER-IV: CHEMICAL GROUP THEORY, SPECTROSCOPY &
ERRORS IN CHEMICAL ANALYSIS

Learning Objectives

- To learn about the basic of application of mathematical concepts to Chemistry.
- To know the experimental errors in chemical analysis concepts Chemistry
- To understand the of spectroscopic methods of chemistry

UNIT – I : Chemical Group Theory

UNIT- II : Fundamentals of Spectroscopy & Microwave Spectroscopy

UNIT- III : Mossbauer Spectroscopy

UNIT –IV :Errors in Chemical Analysis

UNIT – I : Chemical Group Theory: 15 Hours (1 Credit)

Symmetry elements and symmetry operations; Point groups; Mathematically requirements for a point group; Schoenflies notations of point groups; Systematic assignment of molecules to point groups; Group generating elements; sub-groups; Classes; Matrix representation of C_{2V} , C_{3V} and C_{4V} point groups; Reducible and Irreducible representations (IR), Character of a matrix, characters of conjugate matrices; Character of a representation; Properties of Irreducible representation; construction of Character tables (C_{2V} and C_{3V} point groups); Mullikan symbolism rules for IR's; The standard reduction formula: The direct product; Symmetry of normal modes of molecules (C_{2V}).

UNIT-II: Fundamentals of Spectroscopy & Microwave Spectroscopy: 15Hours(1 Credit)

Electromagnetic radiation – Interaction of electromagnetic radiation with matter- Absorption and Emission. Quantization of energy- Regions of the electromagnetic spectrum and the mode of interactions with molecules. Representation of spectra. Basic components of a spectrometer. Signal to noise ratio. Intensity and width of spectral lines.

Microwave Spectroscopy: Classification of rotating molecules- Diatomic molecules- rigid rotor mode. Intensity of spectral lines. Effect of isotopic substitution on transition frequencies, intensities, non rigid rotor, polyatomic molecules- Spectra of linear and symmetric top

molecules. Selection rules. Techniques and Instrumentation. Stark Effect, Nuclear and Electron spin interactions and effect of External field. Applications: calculation of bond lengths in diatomic molecule

UNIT-III: Mössbauer Spectroscopy : 15Hours (1Credit)

Principles of Mossbauer spectroscopy, Resonance line shifts or isomer shift, Quadrupole interactions and Magnetic interactions. Instrumentation, Lamb Mossbauer factor, presentation of spectrum, Selection rules. Applications: Low spin, high spin Fe(II) and Fe(III) complexes, diamagnetic and covalent compounds, biological systems, Investigation of dithiocarbamate and Ruthenium complexes, structure determination of $\text{Fe}_3(\text{CO})_{12}$, Nature of chemical bond, detection of oxidation state, Applications Mössbauer spectroscopy to Tin and Iron compounds.

UNIT-IV: Errors in Chemical Analysis & Statistical Evaluation of Data:15 Hours(1 Credit)

Systematic and random errors. Accuracy and precision. Ways of expression accuracy and precision, Normal error curve and its equation, Propagation of error, Useful statistical test: test of significance, the F test, the student 't' test, the chi test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation, comparison of mean with true values, significant figures regression analysis (least-square method for linear plots), statistics of sampling and detection limit evaluation.

Course outcome:

The Chemistry students can learn their concepts with basic mathematical tools in addition to the experimental errors which occurred during analysis. It can help to understand the basics of spectroscopic techniques which can be useful to elucidate the structural information of molecules. After completion of this course student can get a basic platform for the further studies of chemical analysis of molecules.

References:

1. Quantitative inorganic analysis by A.I.Vogel
2. Instrumental methods of analysis by Skoog & West.
3. Analytical Chemistry by Skoog, West and Holler, Harcourt College Publishers, 1996.

4. Vogel's Text Book of Quantitative Inorganic analysis by J. BasettEtalElbs, Longman 1978.
5. Principles of Instrumental analysis by DaskoogSaunders College Publishers, New York 1985.
6. Instrumental Methods of Analysis, 6th Edition- Willard, Merritt, Dean, Settle, CBS Publications, 1986.
7. Chemical Structure and Bonding- R.L. Decock and H.B. Gray.
8. Molecular Structure and Spectroscopy- G. Aruldhas, Prentice Hall of India Pvt. Ltd, New Delhi 2001
9. Modern Spectroscopy- J.M. Hoilas, John Willey
10. Introduction to Molecular Spectroscopy- G.M. Barrow, Mc Graw Hill.
11. Spectroscopic Identification of organic compounds – Silverstein, Basseler and Morrill.
12. Organic Spectroscopy- William Kemp.
13. Fundamentals of Molecular Spectroscopy- C.N.Banwell and E.A. Mc cash 4th Edition, Tata Mc Graw Hill Publishing Co., Ltd. 1994.
14. Physical Methods in Inorganic Chemistry – R.S.Drago, Saunders Publications.
15. Application of Mossbauer Spectroscopy – Green Mood.
16. NMR, NQR, EPR and MÖssbauer Spectroscopy in inorganic chemistry – R.V Parish, Ellis, Harwood.
17. Instrumental Methods of Chemical Analysis- H.Kaur, PragathiPrakashan, 2003.
18. Instrumental Methods of Analysis, 7th Edition – Willard, Merrit, Dean, Settle, CBS Publications, 1986.
19. Molecular Structure and Spectroscopy – G. Aruldhas, Prentice Hall of India Pvt.Ltd, New Delhi, 2001.
20. Mossbauer Spectroscopy – N.N. Green Wood and T.C. Gibb, Chapman, and Hall, Landon 1971.
21. Analytical spectroscopy – Kamlesh Bansal, Campus books, 2008.
22. Structural Inorganic Chemistry MÖssbauer Spectroscopy – Bhide.
23. Principle of MÖssbauer Spectroscopy – T.C. Gibb, Chapman, and Hall, Landon 1976
24. Symmetry and Spectroscopy of Molecules by K. Veera Reddy

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
(Effective from the academic year 2015-2016)
FIRST SEMESTER INORGANIC CHEMISTRY LAB COURSE
Under CBCS

FIRST SEMESTER(Total Marks 100)

Qualitative semi micro Inorganic analysis:

Semi micro qualitative inorganic mixture analysis contain four cautions. The analysis involves identification and conformation of citations containingthe less familiar rare elements such as Tungsten, Molybdenum, Zirconium, Thorium, Titanium, Uranium, Cerium, Vanadium, Lithium, Berkelium Etc...

(A minimum of 4 mixtures are to be analyzed)

RAYALASEEMA UNIVERSITY
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(Effective from the academic year 2015-2016)
FIRST SEMESTER ORGANIC CHEMISTRY LAB COURSE
Under CBCS

FIRST SEMESTER LAB COURSE (Total Marks 100)

I) Laboratory techniques (For Demonstration Purpose only), Determination of Melting Point /Boiling Point, Ordinary Distillation, Vacuum distillation/filtration, Recrystallization, Drying of Organic Compounds, TLC analysis, Column Chromatography

II) Qualitative Systematic Analysis of single Organic compound,

III) Preparation of single step organic compounds

- i) Aspirin from salicylic acid (Acetylation)
- ii) β -naphthylmethylether (Methylation)
- iii) Iodoform
- iv) Diels-Alder Reaction

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
(Effective from the academic year 2015-2016)
FIRST SEMESTER PHYSICAL CHEMISTRY LAB COURSE
Under CBCS

FIRST SEMESTER (Total Marks 100)

Instrumental methods of Analysis

Conductometry

Titration of strong acid vs strong base (HCl vs NaOH)

Titration of weak acid vs strong base (AcOH vs NaOH)

Titration of mixture of acids (HCl + AcOH) Vs strong base (NaOH)

Potentiometry

Titration of a strong acid vs strong base (HCl vs NaOH)

Titration of weak acid vs strong base (AcOH vs NaOH)

Redox titration (Fe^{2+} Vs $\text{K}_2\text{Cr}_2\text{O}_7$)

Colorimetry

Determination of wavelength of maximum absorbance of a colored solution

Verification of Beers Lambert's law and estimation of given unknown.

Department of Chemistry: Semester II

RAYALASEEMA UNIVERSITY: KURNOOL
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
II Semester under CBCS
(Effective from the academic year 2015-2016)

S.No	Paper Number	Title of Paper	No. Of Credits	Univ. Exam Duration(Hrs)	Total Marks	
					IA	SEE
1	CHEM-OC/NP201: Paper I	Inorganic Chemistry -II (Common to OC & NP)	4	3	30	70
2	CHEM OC/NP202: Paper II	Organic Chemistry-II (Common to OC & NP)	4	3	30	70
3	CHEM OC/NP203: Paper III	Physical Chemistry – II (Common to OC & NP)	4	3	30	70
4	CHEM OC/NP204:Paper IV	Organic Spectroscopy (Common to OC & NP)	4	3	30	70

IA : Internal Assessment = IAE (25) + SS (5)

SEE : Semester End Examination

IAE : Internal Assessment Examination

SS : Student Seminar

RAYALSEEMA UNIVERSITY: KURNOOL
M Sc., ORGANIC CHEMISTRY (OC)/NATURAL PRODUCTS (NP)
II SEMESTER SYLLABUS under CBCS
(EFFECTIVE FROM THE ACADEMIC YEAR 2015-2016)
CHEM-OC/NP: 201: PAPER-I INORGANIC CHEMISTRY –II

UNIT –I : Reaction mechanisms of complexes

UNIT–II: Electronic spectra of transition metal complexes

UNIT-III: Metal-Carbonyl clusters

UNIT-IV: Bioinorganic Chemistry

Learning Objectives

- To discuss basic principles of reaction mechanism in complexes
- To understand electronic spectra of transition metal complexes and to discuss configurations
- To introduce metal carbonyl clusters and to understand LNCCS and HNCCS and their structures
- To discuss the structures and functional aspects of Chlorophylls, Myoglobin and Hemoglobin

UNIT-I : Reaction mechanisms of complexes: 15Hours (1Credit)

Reactivity of metal complexes, inert and labile complexes, Kinetics and mechanisms of substitution reactions, kinetics of substitution reactions in octahedral complexes, acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Anation reactions, substitution reactions in square planar complexes, Trans effect, Mechanism of trans effect, Electron transfer reactions, inner sphere and outer sphere mechanisms, Marcus theory.

UNIT-II: Electronic spectra of transition metal complexes: 15Hours (1Credit)

Free Ion terms and Energy Levels: Configurations, Terms, States and Microstates, calculation of Microstates for P^2 and d^2 Configuration, L-S (Russell- Saunders) Coupling Schemes, J-J Coupling scheme, derivation of terms for P^2 and d^2 configuration. Hole Formulation, Energy ordering of terms (Hund's Rules), Selection rules: Laporte orbital selection rule, spin selection rules. Splitting of energy levels and spectroscopic states Orgel diagrams of d^1 to d^9 metal complexes. Interpretation of electronic spectra of aquo Complexes of Ti(III), V(III), Cr(III), Mn(II), Fe(II), Fe(III), Co(II), Ni(II) and Cu(II). Calculation of interelectronic and spectral

parameters for d^8 metal complexes. Tanabe- Sugano diagrams for d^2 and d^6 octahedral complexes. Charge transfer ($L \rightarrow M$ and $M \rightarrow L$) spectra of metal complexes.

UNIT-III: Metal-Carbonyl Clusters: 15Hours (1Credit)

Anionic and hydrido clusters . Low nuclearity clusters (LNCCs) (Triatomic and tetra atomic). Isoelectronic and isolobal relationships. Structural patterns of high nuclearity carbonyl clusters (HNCCs) Electron counting Schemes of HNCCs- Wades rules. The capping rule. HNCCs of the Fe, Ru, and Os group. HNCCs of Co, Rh and Ir group, HNCCs Ni, Pd and Pt; Octahedral metal halide and chalcogenide clusters , Chevrel phases, compounds with M-M multiple bonding, Major structural types (Edge sharing bi-octahedra, face sharing bi-octahedra, tetragonal prismatic and trigonal antiprismatic structure)-Quadruple bond, One dimensional solids.

UNIT-IV: Bioinorganic Chemistry : 15Hours (1Credit)

- i) Essentials and trace elements in biology: Classification, concept of essential, Evolution of essential trace elements, Role of Bulk (structural) elements and minerals, working of essential trace elements, Deficiency signs and specific function of essential trace elements (Fe, Cu, Co, Ni, Zn, F, I, Se). Antagonism and synergism among essential trace elements.
- ii) Oxygen uptake proteins Structural and functional aspects of Hemoglobin(Hb), Myoglobin(Mb), Hemerythrin(He) and Hemocyanine(Hc). Oxygen binding curves for Hb and Mb, structure-function relationships.
- iii) Photosynthesis: Structure of Chlorophyll, photosynthesis in bacteria and in green plants (Z-scheme involving PS I & PS II).

Course outcome:

- Understanding the importance of trace elements in biology
- Explain selection rules, Tanabe-Sugano diagrams. Orgel diagrams
- Explain the kinetics of substitution reaction, conjugate base mechanism and trans effect

References:

1. Symmetry and Spectroscopy of Molecules, by K. Veera Reddy, New Age International Publishers, New Delhi, 1998.
2. Concise Inorganic Chemistry by J. D. Lee, ELBS, 4th edition, 1994.
3. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson, 5thEdn., John Wiley and Sons, New York.
4. Inorganic Chemistry by J. E. Huheey, E.A. Keiter and R.A. Keiter, 4th edition, Addison Wesley Publishing Company, New York, 2000.
5. Bioinorganic Chemistry, R.W. Hay, Ellis Horwood Ltd., Chichester, New York. 1984.
6. Bioinorganic Chemistry, K. Hussain Reddy, New Age International Publishers, New Delhi, 2003.
7. Reaction Mechanism of metal complexes, Robert W. Hay, Harwood Publishers, Chichester, England, 2000.
8. Inorganic Reaction Mechanisms, M.L. Toba and John Burgess, Addison Wesley, Longman, 1999.
9. Mechanism of Reactions in transition metal sites, Richard A. Henderson, Oxford Science Publications, London, 1993.
10. Kinetics and Mechanisms of Reactions of Transition metal complexes, R.G. Wilkins, 2nd Ed., V.C.H. Publications, 1991.
11. Mechanisms of Inorganic Reactions, F. Basalo and R.G. Pearson, Wiley Easter, 2nd Ed., 1997.
12. Inorganic Electronic Spectroscopy by A. B.P. Lever Elsevier

RAYALSEEMA UNIVERSITY: KURNOOL
M Sc., ORGANIC CHEMISTRY (OC)/NATURAL PRODUCTS (NP)
II SEMESTER SYLLABUS under CBCS
(EFFECTIVE FROM THE ACADEMIC YEAR 2015-2016)
CHEM-OC/NP: 202: PAPER-II ORGANIC CHEMISTRY –II

UNIT- I: Reactive Intermediates and Molecular Rearrangements

UNIT – II: Pericyclic Reactions

UNIT-III: Reagents of Synthetic Importance (Oxidations & Reductions)

UNIT-IV :Heterocyclic Compounds

Learning Objectives

- To discuss pericyclic reactions
- To develop interest in reactive intermediates, molecular rearrangements
- Explain the importance of oxidations, reductions and organometallic reagents

UNIT- I: Reactive Intermediates and Molecular Rearrangements: 15Hours(1Credit)

Reactive intermediates- Generation, Structure and stability of (i) carbocations, (ii) carbanions, (iii) carbenes, (iv) nitrenes and (v) free radicals.

Molecular rearrangements: Definition & Classification, Molecular rearrangements involving (i) electron deficient carbon Wagner-Meerwein, Pinaco-Pinacolone and Wolf rearrangements. (ii) Electron deficient nitrogen; Hoffman, Lossen, Curtis, Schimdt and Beckmann rearrangements. (iii) Electron deficient oxygen Baeyer-villegger oxidation.

Base catalyzed rearrangements, Benzilic acid rearrangement, Favorskii rearrangement, Trans annular and Sommllett-Hauser rearrangement.

UNIT – II: Pericyclic Reactions : 15Hours(1Credit)

Molecular orbital symmetry. Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene. Classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motions. $4n$, $4n + 2$. Cyclo additions – antarafacial and suprafacial additions, $4n$, and $4n + 2$.

Sigmatropic rearrangements – suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3-sigmatropic rearrangements. Claisen, cope and aza-Cope rearrangements.

Unit-III: Reagents Of Synthetic Importance (OxidationsReductions) : 15Hours(1Credit)

- (a) Oxidations: (i) Alcohols to carbonyls:Cr (VI) oxidants, Swern oxidation, SilverCarbonate. (ii) Prevost and Woodward oxidation. (iii) Oxidations of allylic and benzylic C-H bonds: DDQ and SeO₂.
- (b) Reductions: (i) Catalytic hydrogenation: Homogeneous hydrogenation-Use of Wilkinsons catalyst. (ii) Dissolving metal reductions including Birch reduction. (iii) Nucleophilic metal hydrides: LiAlH₄, NaBH₄, and their modifications. Electrophilic metal hydrides : BH₃, and AlH₃. (iv) Hydrogenolysis, use of tri-n-butyltin hydride.
- (c) Organometallic reagents: Preparation and application of the following in organic synthesis : (i) Organo lithium and Organo copper reagents. (ii) Organo boranes in C—C bond formation.

UNIT-IV:Heterocyclic Compounds: 15Hours(1Credit)

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms. Synthesis and reactivity of Indole, Benzofuran, Benzothiophene, Quinoline, Isoquinoline, Coumarin, Chromone, and Acridine.Synthesis and reactivity of the following Heterocycles : 1,2,3-triazole, 1,2,4-triazole, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,3-thiadiazole, 1,2,3-triazine.Synthesis and reactivity of benzodiazepines, benzooxepines and benzothieepines.

Course outcome:

- Basic ideas of the heterocyclic compound, their importance and synthesis
- Applications of organic metallic compounds in the synthesis
- The generation, structure and stability of reactive intermediates in organic reactions

References:

1. Conservation of orbital symmetry by Woodward and Hoffmann
2. Organic reactions and orbital symmetry by Gilchrist and Storr
3. Pericyclic reactions—a problem solving approach by Lehr and Merchand
4. Pericyclic reactions by Mukherjee
5. Mechanism and structure in organic chemistry by S, Mukherjee
6. Some modern methods of organic synthesis by W. Carruthers
7. Guide book of organic synthesis by R. K. Meckie, D. M. Smith & R. A. Atken
8. Reagents in organic synthesis by B. P. Munday and others
9. Organic synthesis by O. House
10. Organic synthesis by Michael B. Smith
11. Reagents for organic synthesis by Fieser&Fieser, Vol. 1-11 (1984)
12. Hand book of reagents for organic synthesis by Reich and Rigby Vol. I & IV
13. Organic Synthesis by Robert E Ireland
14. The third dimension in organic chemistry by Alan Bassindale
15. Stereochemistry of carbon compounds by Ernest L. Eliel
16. Stereochemistry by V. M. Potapov
17. Stereochemistry of Organic compounds- Principles and Applications by D. Nasipuri
18. Stereochemistry, Conformational and Mechanism By P. S. Kalsi.
19. Heterocyclic chemistry, T. L. Gilchrist, Longman UK Ltd., London(1985)
20. Heterocyclic chemistry, 3rdEdn. J. A. Joule, K. Mills and G. F. Smith, Stanley Thornes Ltd., UK, (1998)
21. The Chemistry of Indole, R. J. Sunderberg, Academic Press, New York (1970)

RAYALSEEMA UNIVERSITY: KURNOOL
M Sc., ORGANIC CHEMISTRY (OC)/NATURAL PRODUCTS (NP)
II SEMESTER SYLLABUS under CBCS
(EFFECTIVE FROM THE ACADEMIC YEAR 2015-2016)
CHEM-OC/NP: 203: PAPER-III PHYSICAL CHEMISTRY –II

Learning Objectives

- To learn about the phase rule and its applications to various components.
- To understand the theoretical models and application for the systems under investigation.
- To derive the Phase rule, Michales – Menton Kinetics, energy of Particle in a box. One dimensional and three dimensional and Debye Huckelonsagar equation.

UNIT – I: Thermodynamics – II

UNIT – II: Electro Chemistry – II

UNIT- III: Quantum Chemistry – II

UNIT – IV: Chemical Kinetics – II

UNIT – I: Thermodynamics – II: 15Hours(1Credit)

- A. Phase equilibria: Equilibrium between two phases of one component. The Clapeyron equation. The ClausiusClapeyron equation. Applications. Integrated form of Clapeyron equation.
- B. Phase rule: Thermodynamic derivation of phase rule – Systems of two components. Simple eutectic. Azeotropes. Thermal analysis. Three component systems (Two salts and water). Roozeboom plots.
- C. The equilibrium constant: Equilibrium in homogeneous gaseous systems. Free energy change in chemical reactions. Vant' Hoff's reaction isotherm. Integrated form. Direction of chemical change. Determination of Standard free energies.

UNIT – II: Electro Chemistry – II : 15Hours(1Credit)

- A. Concept of activity and activity coefficient of an electrolyte. The mean ionic activity coefficient. Calculation of mean ionic activity coefficients. Debye Huckel theory of solutions. Debye Huckel Limiting law and its verification.

- B. Electrode polarization – Decomposition potential and over voltage. Influence of C.D. on over voltage. Influence of P^H on over voltage, influence of temperature on over voltage – Theories of over – voltage. Hydrogen over – voltage.
- C. The Deposition and corrosion of metals: Physical nature of electrodeposited metals – 1) Current density 2) Concentration of electrolyte 3) Temperature 4) Colloidal matter 5) Electrolyte 6) Basis metal. Throwing power separation of metals by electrolysis. Electrochemical passivity. Theories of passivity. Corrosion of metals. Hydrogen evolution type.

UNIT – III: Quantum Chemistry – II : 15Hours(1Credit)

- A. Particle in a box. One dimensional and three dimensional. Plot of Ψ and Ψ^2 – Discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles. Calculations using wave functions of the particle in a box – Normalisation and orthogonality, measurability of energy, position momentum, average values and probabilities. Application of the spectra of conjugated molecules.
- B. Schrodinger equation for the Hydrogen atom – Separation of variables. Quantum numbers n, l and m. Hydrogen like wave functions. Complete wave function angular and radial functions. Radial distribution functions. Hydrogen like orbitals and their representation – Polar plots, Contour plots and boundary diagrams.

UNIT – IV: Chemical Kinetics – II : 15Hours(1Credit)

- A. Homogeneous catalysis. Mechanism of catalysis. Equilibrium treatment. Steady state treatment. Acid base catalysis: Mechanism of acid base catalysis. Catalysis by enzymes. Influence of P^H . MicholisMenton law. Influence of temperature. Examples. Decomposition of acetaldehydecatalysed by Iodine. Catalysed decomposition of hydrogen peroxide.
- B. Free radicals in chemical reactions. Hydrogen oxygen reaction. Upper and lower explosion limits. Heterogeneous reactions. Bimolecular reactions. Adsorption. Langmuir adsorption isotherm. Electronic theories of chemisorption and heterogeneous catalysis.
- C. Introduction to enzyme catalysis. Michales – Menton Kinetics – Effect of pH and effect of temperature on the rates of enzyme reactions.

Course Outcome:

Students can understand the derivation of important concepts and apply to the various system to be investigated. It can provide a way to apply the theoretical knowledge to order to derive the various physical phenomena and to know the effect of pH, temperature on the rates of reactions. Students can acquire the complete conceptual knowledge of physical chemistry.

References:

1. A Text Book of Thermodynamics by Rajaram and Kuriakose.
2. Thermodynamics for Chemistry by S. Glasstone.
3. Text Book of Physical Chemistry by Levine.
4. Electrochemistry by S. Glasstone.
5. Quantum Chemistry by Hanna.
6. quantum Chemistry by A.K. Chandra
7. Chemical Kinetics by K.J. Laidler.

RAYALSEEMA UNIVERSITY
M Sc., ORGANIC CHEMISTRY (OC)/NATURAL PRODUCTS (NP)
II SEMESTER SYLLABUS under CBCS
(EFFECTIVE FROM THE ACADEMIC YEAR 2015-2016)
CHEM-OC/NP: 204: PAPER-IV: Organic Spectroscopy

UNIT – I: UV - Visible Spectroscopy, ORD & CD

UNIT –II: IR & Raman spectroscopy

UNIT –III: ¹H NMR & ESR spectroscopy

UNIT- IV: Mass Spectrometry

Learning Objectives

- To learn about the basics of various spectroscopic techniques
- To understand the instrumentation of spectroscopic techniques.
- To apply the spectroscopy knowledge for the structural elucidation of organic molecules

UNIT -I: UV - Visible Spectroscopy, ORD & CD 15 Hrs(1Credit)

UV and visible spectroscopy: Various electronic transitions (185-800nm), effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

ORD : α -Axial haloketone rule and octant rule – Application of these rules in the determination of absolute configuration of cyclohexanones, decalones and cholestanones.

Circular Dichroism : Principle – positive and negative cotton effects – Absolute configuration

UNIT -II: IR & Raman Spectroscopy 15 Hrs(1Credit)

IR Spectroscopy: Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (Ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FT-IR.

Raman Spectroscopy: Characteristic frequencies of functional groups – Applications to identification of organic molecules-comparison of IR and Raman spectroscopy.

UNIT –III: A. ^1H NMR spectroscopy 15 Hrs(1Credit)

Nuclear spin, nuclear resonance, Saturation shielding of magnetic nuclei, chemical shifts and its measurements, factors influencing chemical shift, deshielding. Spin-spin interactions, factors influencing coupling constants 'J' classification (ABX, AMX, ABC, A_2B_2 etc.), spin decoupling, basic ideas about instrument, FT-NMR, advantages of FT-NMR

Applications of ^1H NMR : Shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (First order spectra), virtual coupling, Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, nuclear Overhauser effect (NOE).

^{13}C NMR Spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants.

B) ELECTRON SPIN RESONANCE SPECTROSCOPY

Basic Principles, Theory of ESR, Comparison of NMR & ESR. Instrumentation, Factors affecting the 'g' value, determination of 'g' value. Isotropic and Anisotropic constants. Splitting hyper fine splitting coupling constants. Line width, Zero field splitting and Kramer degeneracy. Crystal field splitting, Crystal field effects. Applications:- Detection of free radicals; ESR spectra of (a) Methyl radical (CH_3^\cdot), (b) Benzene anion (C_6H_6^-)

UNIT -IV: Mass Spectrometry 15 Hrs(1Credit)

Introduction, principle, instrumentation, single and double focusing mass spectrophotometer, Ionisation Methods EI, CI, FD, FAB Factors affecting fragmentation ion analysis, ion abundance, Molecular-ion peak, Nitrogen rule, Base peak, Metastable ion, Isotopic abundance, McLafferty rearrangement. Mass spectral fragmentation patterns of various classes of organic

compounds, Alkanes, cyclo alkanes, alkenes, aromatic hydrocarbons, Aliphatic, Aromatic, Aldehydes, Ketones, Alcohols, phenols, aliphatic Aromatic Nitro Compounds Nitrites, Nitrates, Nitriles.

Course Outcome:

Students can understand the fundamentals of spectroscopic techniques and apply to investigate the structural information of molecules. It can provide a platform to get the awareness towards UV, FTIR, Raman, ^1H NMR and Mass Spectrometry which aims to apply these knowledge towards research.

REFERENCE BOOKS:

1. Electron Spin Resonance Elementary Theory and Practical Applications- John E. Wertz and James R. Bolton, Chapman and Hall, 1986.
2. Spectroscopic Identification of organic compounds – Silverstein, Basseler and Morrill.
3. Organic Spectroscopy- William Kemp.
4. Fundamentals of Molecular Spectroscopy- C.N.Banwell and E.A. Mc cash 4th Edition, Tata Mc Graw Hill Publishing Co., Ltd. 1994.
5. Physical Methods in Inorganic Chemistry – R.S.Drago, Saunders Publications.
6. Application of Mössbauer Spectroscopy – Green Mood.
7. NMR, NQR, EPR and Mössbauer Spectroscopy in inorganic chemistry – R.V Parish, Ellis, Harwood.
8. Instrumental Methods of Chemical Analysis- H.Kaur, PragathiPrakashan, 2003.
9. Instrumental Methods of Analysis, 7th Edition – Willard, Merrit, Dean, Settle, CBS Publications, 1986.
10. Molecular Structure and Spectroscopy – G. Aruldas, Prentice Hall of India Pvt.Ltd, New Delhi, 2001.
11. Mössbauer Spectroscopy – N.N. Green Wood and T.C. Gibb, Chapman, and Hall, Landon 1971.
12. Coordination Chemistry: Experimental Methods- K. Burger, London Butter Worths, 1973.
13. Analytical spectroscopy – Kamlesh Bansal, Campus books, 2008.
14. Structural Inorganic Chemistry Mössbauer Spectroscopy – Bhide.
15. Principle of Mössbauer Spectroscopy – T.C. Gibb, Chapman, and Hall, Landon 1976.

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
(Effective from the academic year 2015-2016)
SECOND SEMESTER INORGANIC CHEMISTRY LAB COURSE
Under CBCS

SECOND SEMESTER

Quantitative Inorganic analysis:

- A. 1. Estimation of zinc in presence of copper
2. Estimation of nickel by gravimetry using DMG

B. Preparations of Inorganic Complexes

1. Preparation of tetra ammine Cu (II) sulfate
2. Preparation of Hexa ammine Ni (II) chloride.
3. Preparation of Potassium tri Oxalato Chromate (III)
4. Mercuric tetrathiocyanato Cobaltite (II)

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
(Effective from the academic year 2015-2016)
SECOND SEMESTER ORGANIC CHEMISTRY LAB COURSE
Under CBCS

SECOND SEMESTER LAB COURSE (Total Marks 100)

I) Separation of two component mixtures by chemical methods and their identification by chemical reactions. Separation by using solvent water, Ether, 5% aq. sodium bicarbonate, aq. 5% sodium hydroxide, and 5% aq. hydrochloric acid solutions. Identification of each compound by a systematic study of the physical constants M.P/B.P, extra elements (Nitrogen, Halogen), Solubility, Functional groups and preparation of crystalline derivatives

Note: As minimum of 5 mixtures should be separated and analyzed by these procedures

II) Multi step synthesis of Organic compounds

- i) Beckmann rearrangement: Benzophenone → Benzophenone oxime → Benzanilide
- ii) Benzilic acid rearrangement : Benzoin → Benzil → Benzilic acid
- iii) Acetylation: Aniline → Acetanilide → ParabromoAcetanilide
- iv) Perkin Reactions : Preparation of Cinnamic acid

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
(Effective from the academic year 2015-2016)
SECOND SEMESTER PHYSICAL CHEMISTRY LAB COURSE
Under CBCS

SECOND SEMESTER (Total Marks 100)

Distribution

Distribution of acetic acid between n-butanol and water.

Distribution of iodine between CCl_4 and water.

Distribution of benzoic acid between Benzene and water & to prove dimerization of benzoic acid in benzene.

Chemical Kinetics

Acid catalysed hydrolysis of methyl acetate & to determine the relative strengths of acids.

Rast's Method

Determination of cryoscopic constant using known solute.

Determination of molecular weight of unknown nonvolatile solute.

Adsorption

Adsorption of acetic acid or Oxalic acid on the surface of charcoal and verification of Freundlich Adsorption isotherm

Critical Solution Temperature (CST)

Determination of CST of Phenol water System

Effect of Neutral Salt on CST

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
III Semester under CBCS
(Effective from the batch admitted during the academic year 2015-2016)

S.No	Paper Number	Title of Paper	No. Of Credits	Uni.Exam Duration(Hrs)	Total Marks	
					IA	SEE
1	CHEMOC/NP301: Paper I	Modern Organic Synthesis (Common to OC & NP)	4	3	30	70
2	CHEMOC/NP302: Paper II	Asymmetric Synthesis and Organic Photochemistry (Common to OC & NP)	4	3	30	70
3	CHEMOC/NP303: Paper III	Bio-Organic Chemistry(Common to OC & NP)	4	3	30	70
4	CHEMOC/NP304: Paper IV	Advanced Organic Spectroscopy(Common to OC & NP)	4	3	30	70

IA : Internal Assessment = IAE (25) + SS (5)

SEE : Semester End Examination

IAE : Internal Assessment Examination

SS : Student Seminar

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
Syllabus for III Semester under CBCS
(Effective from the batch admitted during the academic year 2015-2016)
CHEM-OC/NP301: Paper I – Modern Organic Synthesis

- UNIT –I : Organo Phosphorous and Organo Sulphur Compounds**
UNIT –II : New synthetic reactions
UNIT –III : New techniques and concepts in organic synthesis:
UNIT –IV : Synthetic Strategies
-

Learning Objectives

- To develop familiarity with Arbusov reactions, Perkov reactions and Wittig's reactions
- To discuss the protecting groups with example
- To discuss named reactions
-

UNIT -I: OrganoPhosphorousand Organo Sulphur Compounds 15 Hrs (1 Credit)

Properties of divalent sulphur and trivalent phosphorous derivatives, nucleophilic reactivities, hard and soft acids and bases, compounds containing phosphorous-oxygen bonds, the phosphoroyl group, molecules with hydrogen bonded to phosphoroyl group, Arbusov reactions, Perkov reactions, compounds containing sulphur-oxygen bonds, sulfoxides and sulfones-Pummerer rearrangements, sulfoxides as oxidizing agents, phosphorous ylides, Wittig's reactions and mechanism, the Emmons-Wadsworth reaction, reactions of sulphur ylides.

UNIT -II: New synthetic reactions 15 Hrs (1 Credit)

- (i)Protecting Groups: (a) Protection of alcohols by ether, silyl ether and ester formation
(b) Protection of 1,2-diols by acetal, ketal and carbonate formation (c) Protection of amines by acetylation, benzylation, benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups, (d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups,
(e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.
- (ii)Baylis-Hillman reaction, RCM olefm metathesis, . Stork-enamine reaction and Umpolung use of dithio acetals

UNIT -III: New techniques and concepts in organic synthesis 15 Hrs(1 Credit)

Solid phase polypeptide synthesis, Solid phase oligonucleotide synthesis, Strategies in oligosaccharide synthesis, Kahneglycosidation, Combinatorial synthesis, Phase transfer catalysis, Tandem synthesis, Baldwin rules, Chiron approach in synthesis, Transformations using esterases

and lipases, Determination of absolute configuration (R/S) using Mosher's method and Felkin-Anh model. Use of protecting groups in organic synthesis: fmoc, t-BOC, TBDMS and THP.

UNIT -IV: Synthetic Strategies 15 Hrs(1 Credit)

Synthetic Strategies, Terminology: target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. Strategic bond: Criteria for disconnection of strategic bonds. Importance of the order of events in organic synthesis. One group and two group C-X disconnections. One group C-C disconnections. Alcohol and carbonyl compounds. Two group C-C disconnections; DielsAlder reaction, 1,3-difunctionalised compounds, Control in carbonyl condensation, 1,5- difunctionalised compounds, Michael addition and Robinson annulation, synthesis of (+) Disparlure by retro synthetic approach.

Course outcome:

- Applying synthetic strategies in the synthesis of organic compounds
- Explaining new techniques and concepts in organic synthesis
- Discussing the mechanism of organic reactions

Recommended Books:

1. Some modern methods of organic synthesis by W Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic synthesis by O House
4. Organic synthesis by Michael B Smith
5. Reagents for organic synthesis, by Fieser&Fieser, Vol 1-11(1984)
6. Organic synthesis by Robert E Ireland
7. Organic Synthesis - The disconnection approach by S Warren
8. Organic Synthesis by C Willis and M Willis
9. Handbook of reagents for organic synthesis by Reich and Rigby, Vo I, IV
10. Problems on organic synthesis by Stuart Warren
11. Total synthesis of natural products: the Chiron approach by S.Hanessian
12. Organic chemistry Claydon and others 2005
13. Name Reactions by Jie Jack Li
14. Reagents in Organic synthesis by B.P.Mundy and others.
15. Tandem Organic Reactions by Tse-Lok Ho
16. Advanced Organic Chemistry-Reactions and Mechanism, 2nd Ed. By Bernard Miller and Rajendra Prasad (Pages 397-414)

Department of Chemistry: Semester III

RAYALASEEMA UNIVERSITY

M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP) Syllabus for III Semester

(Effective from the batch admitted during the academic year 2015-2016)

CHEM-OC/NP302: Paper II –Asymmetric Synthesis and Organic Photochemistry

- UNIT –I : Asymmetric Synthesis-I
UNIT –II : Asymmetric Synthesis-II
UNIT –III : Organic Photochemistry - I
UNIT – IV : Organic Photochemistry -II

Learning Objectives

- To explain basics of asymmetric synthesis and organic photochemistry
- To discuss conformational analysis

UNIT –I: Asymmetric Synthesis-I: 15 Hrs (1 Credit)

Introduction and terminology: Topocity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Selectivity in synthesis: Stereospecific reactions (substrate stereoselectivity). Conditions Stereoselective reactions (product stereoselectivity): Enantioselectivity and diastereoselectivity.: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity. Analytical methods: % Enantiomer excess, optical purity, % diastereomeric excess. Techniques for determination of enantioselectivity: Specific rotation, Chiral ¹H nmr, Chiral lanthanide shift reagents and Chiral HPLC.

UNIT -II: Asymmetric Synthesis-II: 15 Hrs (1 Credit)

i) Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1,2- asymmetric induction, Cram's rule and Felkin-Anh model.

ii) Chiral auxiliary controlled asymmetric synthesis: α -Alkylation of chiral enolates, azaenolates, 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder and Aldol reactions.

iii) Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC₂ BH and IPCBH₂. Reductions with CBS reagent.

iv) Chiral catalyst controlled asymmetric synthesis: Sharpless, Jacobsen and Shi asymmetric epoxidations. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalysts, Enzyme mediated enantioselective synthesis:

UNIT-III :Organic Photochemistry – II15 Hrs (1 Credit)

Organic photochemistry : Molecular orbitals, carbonyl chromophore–triplet states, Jablonski diagram, inter–system crossing. Energy transfer. Energies properties and reaction of singlet and triplet states of and transitions.

Photochemical reactions : (a) Photoreduction, mechanism, influence of temperature, solvent, nature of hydrogen donors, structure of substrates on the course of photo reduction, (b) F.B. reaction mechanism, stereochemistry, side reaction due to variations of the triplet energy of the carbonyl component and the nature of the olefin component.

UNIT – IV: Organic Photochemistry – II15 Hrs (1 Credit)

Norrish cleavages, type I : Mechanism, acyclic cyclicdiones, influence of sensitizer, photo Fries rearrangement. Norrish type II cleavage : Mechanism and stereochemistry, type II reactions of esters : 1: 2 diketones, photo decarboxylation. Photochemistry of unsaturated ketones – Olefin photochemistry, cyclic olefins – Photochemistry – of conjugated dienes; electrocyclisations, influence of triplet energy of sensitizer, sensitized and unsensitized electrocyclisations. Electrocyclisations of dienes in crossed sense – Photochemistry of benzene derivatives – formation of derivatives of benzavalene, fluvene and Dewar benzene, cyclo addition of benzene to olefins and dienes – Decomposition of nitrites – Barton reaction. Di - π methane rearrangement.

Course outcome:

- Identify applications of asymmetric synthesis
- Basic idea of organic photochemistry

Recommended Books:

1. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
2. The third dimension in organic chemistry, by Alan Bassendale
3. Stereochemistry: Conformation & Mechanism by P S Kalsi
4. Stereochemistry of Carbon compounds by Ernest L Eliel
5. Stereoselectivity in organic synthesis by R S Ward.
6. Asymmetric synthesis by Nogradi
7. Asymmetric organic reactions by it) Morrison and HS Moscher

8. Stereo differentiating reactions by Izumi
9. Some modern methods of organic synthesis by W Carruthers
10. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
11. Organic synthesis by Michael B Smith
12. Molecular Reactions and Photo chemistry by Depuy and Chapman
13. Photochemistry by C W S Wells
14. Organic Photochemistry by Turro
15. Molecular Photochemistry by Gilbert & Baggo
16. Organic Photochemistry by D Coyle

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
Syllabus for III Semester under CBCS
(Effective from the batch admitted during the academic year 2015-2016)
(CHEM-OC/NP303: Paper III – Bio-Organic Chemistry)

Learning Objectives

- To understand recombinant DNA and formation technology
- To explain the mechanism of enzymatic action

UNIT –I : Mechanism of Enzymic action

UNIT –II : Recombinant DNA and Fermentation technology

UNIT –III : Coenzymes

UNIT –IV : Amino acids and Proteins:

UNIT -I: Mechanism of Enzymic action 15 Hrs (1credit)

Transition state theory. Acid-Base catalysis. Co-valent catalysis— Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. Examples of some typical enzyme mechanisms for (i) Triose phosphate isomerase (ii) α -chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease. Synthesis of α - amino acids and peptides. Transformations of lipases and esterases. C-C bond formation: asymmetric cyanohydrin formation and asymmetric aldol condensations using enzymes.

UNIT -II: Recombinant DNA and Fermentation technology 15 Hrs (1credit)

Introduction to genetic engineering. Recombinant DNA technology-restriction endonuclease, cloning, linkers, adaptors. Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples. Principles of finger printing technology- Site directed mutagenesis. Fermentation technology: Introduction to fermentation. Industrial fermentation. Advantages and limitations of fermentation. Production of drugs and drug intermediates from fermentation examples. Chiral hydroxy acids, vitamins, amino acids, β -lactam antibiotics. Precursor fermentation and microbial oxidation and reductions

UNIT -III: Coenzymes 15 Hrs (1credit)

Introduction. Cofactors- cosubstrates- prosthetic groups. Classification-Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of i)

nicotinamide adenosine dinucleotide / their phosphates (NAD⁺, NADH, NADP⁺, NADPH) ii) Flavin adenine dinucleotide FAD, FADH₂ and iii) Flavin mononucleotide (FMN, FMNH₂), lipoic acid, biotin, tetrahydrofolate. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine di phospho sugars (UDP-sugars) Mechanism of reactions catalysed by the above coenzymes.

UNIT-IV:Amino acids and Proteins: (1credit)

Amino acids: Introduction - Classification of amino acids. General methods of preparations – Gabriel’s phthalimide synthesis, Strecker’s synthesis, Malonic ester synthesis Erlenmeyer azalactone synthesis.

Analysis of amino acids from protein hydrolysates. General properties and reactions of amino acids –isoelectric point.

PROTEINS: General nature of proteins – annealing, Biuret reaction, Ninhydrin test. Classification of proteins. Merrified solid phase peptide synthesis. Primary, secondary, tertiary and quaternary structure of proteins.

Course outcome:

- Applying mechanism of reactions catalyzed by coenzymes
- Explaining the importance of amino acids

Recommended Books

1. Concepts in biotechnology by D. Balasubramanian& others
2. Principles of biochemistry by Horton & others.
3. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
4. Chirotechnology by R.Sheldon
5. Organic synthesis in water. By Paul A. Grieco Blackie.
6. Burger’s medicinal chemistry and drug discovery. by Manfred E. Wolf
7. Introduction to Medicinal chemistry. by Graham Patrick.
8. Introduction to drug design. by R.B.Silverman
9. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
Syllabus for III Semester
(Effective from the batch admitted during the academic year 2015-2016)
CHEM-OC/NP :304: Paper IV – Advanced Organic Spectroscopy

UNIT –I	:¹³C NMR Spectroscopy
UNIT –II	: Multipulse techniques in NMR Spectroscopy
UNIT –III	: 2D NMR techniques
UNIT –IV	: Spectral Identification of Natural Products

Learning Objectives

- To learn about the various NMR spectroscopic techniques
- To apply the NMR spectroscopy knowledge for the structural elucidation of organic molecules
- To identify the spectral information of Natural Products Chemistry and Conformational analysis

UNIT –I : ¹³C NMR Spectroscopy 15 Hrs (1credit)

CW and PFT techniques. Types of ¹³C nmr spectra: undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra, signal enhancement by Nuclear OVER HAUSER effect. ¹³C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (¹³C, ¹³C J) and heteronuclear (¹³C, ¹H J and ¹³C- ²H J) coupling. Applications of ¹³C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules.

UNIT -II: Multipulse techniques in NMR Spectroscopy 15 Hrs

Spin echo experiment, ¹³C NMR spectral editing technique, Polarization Transfer and signal enhancement, principle and applications of SPT, APT, INEPT and DEPT methods, 1D-INADEQUATE, Application to Geraniol molecule.

UNIT -III: 2D NMR techniques 15 Hrs (1credit)

2D-NMR techniques:

Principles of 2-D NMR, Classification of 2D-experiments. 2D-J-resolved spectroscopy. Homonuclear and Heteronuclear 2D-J-resolved spectroscopy. Correlation spectroscopy (COSY) Homo COSY (¹H-¹H COSY), TOCSY (Total Correlation Spectroscopy), Hetero COSY (¹H, ¹³C COSY, HMQC), long range ¹H, ¹³C COSY (HMBC), NOESY and 2D-INADEQUATE experiments and their applications.

UNIT -IV:Spectral Identification of Natural Products Chemistry And Conformational Analysis(1credit)

Spectral identification of natural products : Use of spectroscopic methods UV, IR, ^1H and ^{13}C -NMR and Mass spectra in the structure elucidation of natural products. Illustration with suitable compounds like chrysin (flavones). 2,3-dihydroflavone (flavanone), diadzein (isoflavone). Umbelliferone (coumarin), Camphor (Terpenoid) and Papaverine (alkaloid). Cholesterol (steroid).

Course outcome:

- Understanding the concept of NMR Spectroscopy
- Application of NMR Spectroscopy to investigate the spectral identification of natural products

References

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
2. Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
9. Spectroscopy of organic compounds, RM Silverstein and others, 5th Ed, (John Wiley)
10. NMR Spectroscopy An Introduction to Principles, Applications and experimental methods, Joseph B. Lambert and Eugene P. Mazzola (Pearson Education Inc. Prentice – Hall).
11. A Complete Introduction to Modern NMR Spectroscopy, Roger S. Macomber, A (John Wiley & Sons, Inc.).
12. Modern Spectroscopy, M. Hollas (John Wiley)
13. Introduction to molecular Spectroscopy, G. M. Barrow (McGraw Hill)
14. Basic principles of Spectroscopy, R. Chang (McGraw Hill).
15. NMR Spectroscopy by Gunther.
16. NMR Spectroscopy by Attar-ur-Rahman

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
(Effective from the batch admitted during the academic year 2015-2016)
THIRD SEMESTER ORGANIC CHEMISTRY LAB COURSE
Under CBCS

THIRD SEMESTER LAB COURSE-PRACTICAL-III- (Total Marks 100)

Organic Quantitative Estimations

Estimations:

- i) Estimation of phenol.
- ii) Estimation of Glucose.
- iii) Estimation of Aniline.
- iv) Estimation of saponification value of an oil or fat or an ester.
- v) Estimation of acid value of a fat or an oil.

THIRD SEMESTER LAB COURSE-PRACTICAL-IV- (Total Marks 100)

Spectral Identification of Organic Compounds

Spectral Identification of Un-Known Organic Compounds by Interpretation of UV, IR, ^1H NMR, ^{13}C NMR and Mass Spectral Data

Note: A minimum of 30 representative examples should be studied

Recommended Books

1. A text-book of practical organic chemistry by A.I. Vogel, Vol. I and II.
2. Laboratory Manual of Organic Chemistry by B. B. Dey, M. V. Sitaraman Revised by T. R. Govindachari.
3. Unitized experiments in organic chemistry by R.Q. Brewster and others.
4. Practical Organic Chemistry by Mann and Saunders.
5. A textbook of practical organic chemistry by A.I. Vogel, Vol. I and II.
6. Laboratory Manual of Organic Chemistry by B. B. Dey, M. V. Sitaraman Revised by T. R. Govindachari.
7. Unitized experiments in organic chemistry by R.Q. Brewster and others.
8. Practical Organic Chemistry by Mann and Saunders

Department of Chemistry: VI Semester Syllabus

RAYALASEEMA UNIVERSITY
M.Sc. ORGANIC CHEMISTRY (OC) / NATURAL PRODUCTS (NP)
IV Semester under CBCS
(Effective from the batch admitted in the academic year 2015-2016)

S.No	Paper Number	Title of Paper	No. Of Credits	Uni.Exam Duration(Hrs)	Total Marks	
					IAE	SEE
1.	CHEM-OC: 401:Paper-I	Terpenoids, Alkaloids Steroids, and Flavonoids (For OC only)	4	3	30	70
	CHEM-NP: 401:Paper-I	Advanced Natural Products Chemistry (for NP Only)	4	3	30	70
2.	EL-CHEM : OC/NP: 402: Paper II (Common for both OC&NP)	Drug & Medicinal Chemistry And Green Chemistry	4	3	30	70
3.	PROJECT	To be Selected	10	Dissertation	150	
				Viva-Voce	50	
				Total Marks for Project Work	200	

IA : Internal Assessment = IAE (25) + SS (5)

SEE : Semester End Examination

IAE : Internal Assessment Examination

SS : Student Seminar

RAYALASEEMA UNIVERSITY
M.Sc.ORGANIC CHEMISTRY

IV SEMISTER SYLLABUS under CBCS

(Effective from the Batch Admitted In the Academic Year 2015-2016)CHEM: OC: 401:
PAPER-I– TERPENOIDS, STEROIDS, ALKALOIDS AND FLAVONOIDS

UNIT- I: Terpenoids

UNIT - II: Alkaloids

UNIT -III: Steroids

UNIT-IV:Flavonoids&Isoflavonoids

Learning Objectives

- To understand the basic knowledge about naturally occurring compounds
- To develop skill in the synthesis of important compounds

UNIT:I :Terpenoids: 15 hours (1 Credit)

Occurrence, Isolation general methods of structural determination isoprene rule special isoprene rule, structure determination and stereochemistry and synthesis of the following molecules :
1.Santonin 2. Farnesol 3.Zingiberene 4. Cadinene

UNIT II: Alkaloids: 15 hours (1 Credit)

Occurrence, Isolation general methods of structure elucidation and physiological action , degradation , classification based on nitrogen heterocyclic ring , structure, role of alkaloids in plants stereochemistry, synthesis and bio synthesis are the following :

1. Nicotine 2. Morphine 3. Strychnine and 4.Reserpine

UNIT III : Steroids:15 hours (1 Credit)

Occurrence, Isolation general methods of structure elucidation and synthesis of cholesterol (total synthesis not expected) Androsterone, Testosterone , Estrone , Progesterone.

UNIT:IV: Flavonoids And Isoflavonoids:15 Hours (1 Credit)

Occurrence nomenclature and general methods of structure determination, isolation and synthesis of 1. Apigenin, 2. Luteolin, 3. Kaempferol 4. Quercetin 5. Buten, 6.Daidzein. Biosynthesis of Flavonoids and Isoflavonoids: Acetate pathway and shikimic acid pathway.

Course outcome:

- Explain the structure determination and stereochemistry of important compounds.
- Understand the difference between acetate pathway and shikimic pathway

Reference:

1. Comprehensive Organic Chemistry by D.R. Barton and W.D.Ollis.
2. Standard methods in plant analysis by Reach and Tracey.
3. Natural Products by Kalsi.
4. Text book of Organic Chemistry VOL II by I.L.Finar.
5. An Introduction to the Chemistry of terpenoids and Steroids by William Templeton.
6. Systematic identification of flavonoid Compounds by Markhan.&Mabry
7. Steroids by Fieser and Fieser.
8. Alkaloids by Manske.
9. Alkaloids by Bentley.
10. The Chemistry of terpenes by A.R.Pinder.
11. The Terpenes by Simenson.
12. Terpenoids by Mayo

RAYALASEEMA UNIVERSITY
M Sc., NATURAL PRODUCTS
IV SEMESTER SYLLABUS under CBCS
(Effective from the Batch Admitted in the Academic Year 2015-2016)
CHEM-NP: 401: PAPER-I Advanced Natural Products Chemistry

UNIT:I	:	Essential Oils & Oils And Fats
UNIT: II	:	Flavonoids And Isoflavonoids
UNIT III	:	Steroids
UNIT: IV	:	Wood Chemistry

Learning Objectives

- To develop interest to know about the naturally occurring essential oils.
- To explain the structure elucidation of compounds
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UNIT: I:Essential Oils & Oils and Fats 15 hours (1 Credit)

(a)Essential Oils: Occurrence, Isolation and chemical constituents and uses of essential oils 1. Sandalwood oil 2. Lemon grass oil 3. Camphor oil 4. Turpentine oil

(b) Oils and Fats:

Introduction: Distinction between oils and fats. Classification of oils and fats (edible and inedible, non-drying, semi-drying, oil). Analysis of oils and fats; Saponification value, Acid value, iodine value.

UNIT:II: Flavonoids And Isoflavonoids:15 Hours(1 Credit)

Occurrence nomenclature and general methods of structure determination, isolation and synthesis of 1. Apigenin, 2. Luteolin, 3. Kaempferol 4. Quercetin 5. Buten, 6.Daidzein

Biosynthesis of Flavonoids and Isoflavonoids: Acetate pathway and shikimic acid pathway

UNIT III :Steroids: 15 hours(1 Credit)

Occurrence, Isolation general methods of structure elucidation and synthesis of cholesterol (total synthesis not expected) Androsterone, Testosterone , Estrone , Progesterone.

UNIT: IV: Wood Chemistry: 15 hours (1 Credit)

Wood Structure and Chemical composition. Pulp and paper. Chemical pulping (kraft process) Biotechnology –Biopulping and Biobleaching. paper making process. Elements of wood preservation. Additional chemicals from wood. Thermal decomposition of wood. Wood Distillation – pyrolytic acid (production, constituents and industrial uses).

Course outcome:

- Understanding basics of wood chemistry
- Identifying the application of essential oils and fats

Reference Books:

1. Comprehensive Organic Chemistry by D.R. Barton and W.D.Ollis.
2. Standard methods in plant analysis by Reach and Tracey.
3. Natural Products by Kalsi.
4. Text book of Organic Chemistry VOL II by I.L.Finar.
5. An Introduction to the Chemistry of terpenoids and Steroids by William Templeton.
6. Systematic identification of flavonoid Compounds by Markhan.&Mabry
7. Steroids by Fieser and Fieser.

RAYALASEEMA UNIVERSITY
M.Sc.ORGANIC CHEMISTRY (OC)/ NATURAL PRODUCTS (NP)
Syllabus for IV Semester under CBCS
(Effective from the batch admitted in the academic year 2015-2016)

ELECTIVE PAPER

EL-CHEM-OC/NP: 402: Paper II – Drug & Medicinal Chemistry and Green Chemistry

UNIT -I: Principles of Drug design and drug discovery

UNIT -II: Medicinal Chemistry

UNIT -III: Green Chemistry – I

UNIT -IV: Green Chemistry – II

Learning Objectives

- To discuss the principles of drug design and drug discovery
- To introduce green chemistry and microwave assisted reactions

UNIT-I: Principles of Drug design and drug discovery 15 Hrs (1 Credit)

Introduction to drug discovery. Folklore drugs. Natural products as lead structures in drug discovery. Structure pruning technique in lead modification e.g. morphine. Serendipitous discovery of leads e.g. Penicillin and Librium. Drug targets and receptor theory. Nature of drug-receptor interactions. Pharmacodynamics and pharmacokinetics (ADME) of drugs. Agonists, antagonists and enzyme inhibitors. Discovery of lead structure from natural hormones and neurotransmitters. Existing drugs as leads (me too drugs). Principles of design of agonists (e.g. Salbutamol), antagonists e.g. cimetidine) and enzyme inhibitors (e.g. captopril). Principles of prodrug design. Molecular graphics based lead discovery. Introduction to drug patents and Clinical trials.

UNIT-II: Medicinal Chemistry 15 Hrs (1 Credit)

Introduction, sources of natural leads and their structural modification to semi synthetic/synthetic drugs. 1) Drugs acting on nervous system a) CNS: i) morphine alkaloids. Structural pruning technique – eg. Morphine. b) PNS: i) Cocaine, benzocaine, 2) Neuromuscular blocking agents: curare alkaloids, tubocurarine, 3) Anticancer drugs: i) Catharanthus alkaloids, vinblastine, ii) Taxol. 4) Antibiotics: i) β -Lactam antibiotics – penicillin, cephalosporins and their semi synthetic derivatives (amoxicillin, methicillin, cephalexin) 5) Cardiovascular drugs : i) lovastatin 6)

Antiasthma drugs : i) Ephedrine, isoprenaline and salbutamol. 7) Antiparasitic drugs: i) Artemisinin, artemether and artether. ii) Quinine, pamaquine,.

UNIT -III:Green Chemistry - I

Introduction. Principles, atom economy and scope. Introduction to alternative approaches. Solvent free reactions-principle, scope, utility of solvent free conditions, controlling solvent free reactions. Microwave activation-benefits, limitations, equipment, microwave effects- according to reaction medium and according to reaction mechanism. Solvent free microwave assisted organic synthesis: Introduction, solvent free techniques- Reactions on solid mineral supports, solid-liquid phase-transfer catalysts-Reactions without solvent support or catalyst.

UNIT -IV:Green Chemistry - II

Examples of reactions on solid supports, PTC, reactions without support or catalyst— deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions. Microwave assisted reactions in water — Hoffmann elimination, hydrolysis, oxidation, saponification reactions. Microwave assisted reactions in organic solvents — Esterification reactions, Fries rearrangement, OrthoesterClaisen rearrangement, Diels- Alder reaction, decarboxylation. Ultrasound assisted reactions: Introduction, substitution addition, oxidation, reduction reactions.

Course outcome:

- Explaining the discovery of leads and molecular graphics based lead discovery
- Identifying the sources of natural leads and structural pruning technique
- Applying the green synthesis to organic reactions

References

1. Drug design By E.J. Arienes
2. Jenkin's quantitative pharmaceutical chemistry By Knevel and Dryden
3. Recent advances in Bioinformatics by I. A. Khan and A Khanum
4. Molecular modelling By Hans Dieter Holtje and Gerd Folkers
5. Molecular modelling By Leach
6. Bio Informatics by Rastogi
7. The Science and practice of Pharmacy – Vol I and Vol II by Remington

8. Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
9. Introduction to Medicinal chemistry. By Patrick.
10. Introduction to drug design. By Silverman
11. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
12. Principles of medicinal chemistry. By William Foye
13. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
14. New trends in green Chemistry by V.K.Ahluwalia