STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086

M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

ORGANIC CHEMISTRY-I

CODE: 15CH/PC/OC14

CREDITS: 4
L T P: 4 1 0
TOTAL TEACHING HOURS: 65

OBJECTIVES OF THE COURSE

- To understand the importance of the nomenclature of different types of organic compounds and their usage in various reactions
- To enable students to gain knowledge on the various aspects of stereochemistry and to emphasize the importance of stereochemistry in different types of reaction mechanisms
- To understand the methods adopted in the study of reaction mechanisms

Unit 1

Nomenclature of Organic Compounds and Aromaticity (10 hrs.)

1.1 Modern Nomenclature – Cyclic, Acyclic, Aliphatic, Aromatic, Bridged and Heterocyclic Compounds

1.2 Huckel's Rule of Aromaticity, Antiaromaticity, Aromaticity in Annulenes, Diatropic and Paratropic behaviour (in NMR).

1.3 Benzenoid and Non-Benzenoid Aromatics, Homo Aromatic and Pseudoaromatic Compounds

1.4 Aromaticity in Heteroannulenes and Fullerenes

Unit 2

Stereochemistry (18 hrs.)

2.1 Concept of Optical Activity, Chirality, Asymmetry and Dissymmetry. Optical Activity of Allenes, Biphenyls, Spiro Compounds, Cyclobutane, Cyclononane and Molecules with Helical Structures

2.2 Absolute Configuration -D/L and R/S Nomenclature, Assigning R/S Nomenclature to Biphenyls, Allenes and Spiro Compounds, CIP Conventions. Molecules with more than one Asymmetric Centre - Erythro and Threo Nomenclature. Interconversion of Fischer, Sawhorse and Newmann Projection

2.3 Geometrical Isomerism- E-Z Nomenclature of Olefins. Geometrical and Optical Isomerism of Disubstituted Cyclopropane, Cyclobutane and Cyclopentanes. Identification of Enantiotopic, Homotopic, Diastereotopic Hydrogens and Prochiral Carbons in Compounds Containing a Maximum of Ten Carbon Atoms only

2.4 Asymmetric Synthesis- Cram's and Prelog's Rules, Chiral Auxiliaries – Evan Aldol Reaction, Chiral Reagents. Epoxidation (Sharpless' Reaction)

2.5 Stereospeciific and Stereoselective Reactions- Syn and Anti (Addition and Elimination)

Unit 3

Conformations and Conformational Analysis (12 hrs.)

3.1 Conformation and Reactivity in Cyclic Systems - Cyclobutane, Cyclopentane, Cyclohexane, Cycloheptane and Cyclooctane

3.2 Conformational Analysis of Disubstituted Cyclohexanes and their Stereochemical features. Conformation and Reactivity of Cyclohexanols (Oxidation and Acylation), Cyclohexanones (Reduction) and Cyclohexane Carboxylic Acid Derivatives (Hydrolysis)

3.3 Conformation and Stereochemistry of Fused Ring System-Decalins(9 Methyldecalin)

Unit 4

Study of Reaction Mechanisms (15 hrs.)

4.1 Thermodynamic and Kinetic Requirements of Reactions, Energy Profile Diagrams, Intermediate vs Transition State. Hammond Postulates. Curtin-Hammett Principle

4.2 Methods of Determining Reaction Mechanisms-Identification of Products and Intermediates, Cross-Over Experiments, Trapping of Intermediates, Isotopic Labeling, Stereochemical Studies. Kinetic Methods- Kinetic Isotopic Effects, Salt Effects, Solvent Effects-Solvent Isotopic Effects

Unit 5

Structural Effects and Chemical Reactivity (10 hrs.)

5.1 Correlation of Structure with Reactivity. Inductive, Mesomeric, Steric Effects and Steric Inhibition of Resonance

5.2 Quantitative Relationships between Molecular Structure and Chemical Reactivity-Linear Free Energy Relationship - Hammett Equation, Taft Equation, Acidity of Carboxylic Acids and Phenols, Basicity of Aliphatic and Aromatic Bases

TEXT BOOKS

Ahuliwalia V.K. and R.K. Parashar. *Organic Reaction Mechanism***.** New Delhi : Narosa, 2002.

Eliel E.L. *Stereochemistry of Organic Compounds***.** New York : John Wiley, 2003.

Singh, Jagadamba and L.D.S. Yadav. *Advanced Organic Chemistry*. Meerut : Pragati Prakashan, 2010.

Kalsi P.S. *Stereochemistry*. New Delhi: New Age, 2006.

BOOKS FOR REFERENCE

Jonathan Clayden, Nick Greeves and Stuart Warren, *Organic Chemistry*, New York : Oxford University Press, 2012.

Francis A. Carey and Richard J. Sundberg, *Advanced Organic Chemistry Part A: Structure and Mechanisms.* New York : Springer, 2007.

Norman, R.O.C. and J.M.Coxon, *Principles of Organic Synthesis*. New York: CRC Press 2012.

Buxton, S.R. and Roberts S.M. *Guide to Organic Stereo Chemistry*, London: Orient Longman, 1997.

Solomons, T.W Graham. and Craig B. Fryhle. *Organic Chemistry.* NewYork: John Wiley, 2000.

Nasipuri D. *Stereochemistry of Organic Compounds – Principles and Applications,* New Delhi: Wiley Eastern, 1992.

Bansal Raj.K. *Organic Reaction Mechanism*. New Delhi: Tata McGraw-Hill, 2006.

JOURNALS

Tetrahedron letters

Journal of American Chemical Society

Journal of Stereochemistry

WEB RESOURCES

www.oxfordtextbooks.co.uk/orc/clayden2e

www.organic-chemistry.org/reactions.htm

PATTERN OF EVALUATION

Continuous Assessment:

Total Marks: 50 **Duration: 90 mins.**

Section A – 11 x 1 = 11 Marks
(All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 3 x 8 = 24 Marks
(3 out of 4 to be answered)

Section C – 1 x 15 = 15 Marks
(1 out of 2 to be answered)

Third Component:
List of evaluation modes:
Quiz
Seminars
Assignments

END SEMESTER EXAMINATION:

Total Marks: 100 **Duration: 3 hours**

Section A – 20 x 1 = 20 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)
Section B – 5 x 8 = 40 Marks (5 out of 7 to be answered)
Section C – 2 x 20 = 40 Marks (2 out of 3 to be answered)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086
M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS
(Effective from the academic year 2015 – 2016)

ADVANCED PHYSICAL CHEMISTRY

CODE: 15CH/PC/PC14 **CREDITS: 4**
LT P: 4 1 0
TOTAL TEACHING HOURS: 65

OBJECTIVES OF THE COURSE

- To learn to integrate thermodynamics with quantum statistics
- To appreciate and correlate theoretical concepts and experimental details
- To realize the importance of kinetics of chemical transformations and reactions
- To learn the theories of electrolysis
- To encourage a problem solving approach to learning

Unit 1

Statistical Thermodynamics (18 hrs.)

1.1 Introduction to Statistical Mechanics (Permutation, Probability), Microstates, Distributions and the most Probable Distribution, Evaluation of Boltzmann Parameters using Lagrange's Method of Undetermined Multipliers, Stirling Approximation

1.2 Partition Function, Evaluation of Translational, Rotational, Vibrational and Electronic Partition Functions for Ideal Gases, n Particles(Distinguishable and Indistinguishable) Systems

1.3 Applications: Calculation of Thermodynamic Properties in terms of Partition Function, Heat Capacities of Ideal Gases, Heat Capacity of Solids, Residual Entropies, Equilibrium Constant

Unit 2

Quantum Statistics (10 hrs.)

2.1 Bose-Einstein and Fermi-Dirac Statistics, Comparison between Bose-Einstein, Fermi-Dirac and Boltzmann Statistics, Application to Radiation and Electron Gas in Metals

2.2 Irreversible Processes Relating to Mass, Electricity and Heat Exchanges between two Homogenous Isotropic Phases, Phenomenological Equations and Onsager Reciprocity Relation

Unit 3

Molecules in Motion (15 hrs.)

3.1 Accounting for Rate Laws: Simple Reactions, Temperature Dependent on Reaction Rates, Consecutive Reactions(Rate determining Step Approximation and Steady State Approximation), Pre-Equilibria and Unimolecular Reactions- Lindemann-Hinshelwood Mechanism,Kinetics of Complex Reactions- Chain Reactions, Polymerization Reactions, Explosions and Photochemical Reactions

3.2 Molecular Reaction Dynamics: Collision Theory, Steric Factor, Diffusion controlled reactions, Activated Complex Theory, Eyring Equation, Reaction Coordinates and Transition State, Thermodynamic aspects, Reaction between Ions, Effect of Solvent on Reaction Rates, Effect of

Ionic Strength on Reaction Rates (Salt Effects), Dynamics of Molecular Collisions (Molecular Beams), Potential Energy Surfaces

Unit 4

Theories of Electrochemistry (14 hrs.)

4.1 Electrodes and Electrochemical Cells-Evaluation of Thermodynamic Quantities

4.2 The Electrical Double Layer at the Electrode – Electrolyte Interface, Models:Helmholtz Perrin Model, Gouy-Chapmann Model and Stern Model, Potentials (Galvanic and Voltaic) – Theory of Multiple Layer Capacity – Electro- Capillarity – Lippmann Potential – Structure of Double Layers

4.3 Diffusion – Electro Kinetic Phenomena (Electroosmosis, Sedimentation Potential, Electrophoresis, Dorn Effect) – Membrane Potential .I – E Variation –Different Types of Overpotentials – Butler – Volmer Equation for One Electron Transfer (derivation not required) Tafel Plots, Exchange Current Density – Standard Rate Constants – Transfer Coefficient – Tafel and Nernst Equations – Polarisation. Rate Determining Step in Electrode Kinetics – The Hydrogen Overvoltage, Oxygen Overvoltage – Anodic and Cathodic Processes – Redox Reactions, Oxygen-Hydrogen Fuel Cells

Unit 5

Surface Chemistry (8 hrs.)

5.1 Adsorption Isotherms, Types of Adsorption Isotherms, Gibb's Adsorption Isotherm, BET Isotherm (Only Equation) - Determination of Surface Area

5.2 Heterogeneous Catalysis: Catalytic Activity at Surfaces, Adsorption and Catalysis-The Eley-Rideal Mechanism, Langmuir- Hinshelwood Mechanism, Molecular Beam studies, Examples of Catalysis- Hydrogenation, Oxidation, Cracking /Pyrolysis and Reforming

TEXTBOOKS

Castellan, G.W. *Physical Chemistry***.** New Delhi: Addison – Wesley / Narosa, 2004.

Peter Atkins and Jolio de Paula. *Atkins Physical Chemistry***.** Oxford : Oxford Press, 2002

BOOKS FOR REFERENCE

Crow, D.R. *Principles and Applications of Electrochemistry*. New York: CRC Press, 1994.

Nash, K. *Elements of Statistical Thermodynamics*. New York: Dover , 2012.

Gupta,M.C. *Statistical Thermodynamics*, New Delhi: New Age International, 2003.

Dole, M. *An Introduction of Statistical Thermodynamics*, New York: Dover, 1986.

Rajaram J. and Kuriacose J.C. *Kinetics and Mechanism of Chemical Transformations*. New Delhi :Macmillan ,1993.

Kaufmann, E.D. *Advanced Concepts in Physical Chemistry*, New York :McGraw Hill,1966.

Hasse, R. *Thermodynamics of Irreversible Processes*, London: Addison Wesley, 1969.

Barrow Gordon, M. *Physical Chemistry*, Orient Longman : New York, 1977.

Viswanathan B., Sundaram S., Venkataraman R., Rengarajan K., Raghavan P.S. *Electrochemistry– Principles and Applications*, Chennai :Viswanathan ,2007.

Chandler,D. *Introduction to Modern Statistical Mechanics*, Oxford: Oxford University Press, 1997.

McQuarrie, D.A. and Simon, J.D. *Molecular Thermodynamics*, Sansalito: University Science,1999.

Adamson A.W. and Gast, A.P. *Physical Chemistry of Surfaces*, New York :Wiley, 1997.

Lim,Y.K. *Problems and Solutions on Thermodynamics and Statistical Mechanics*, Singapore :World Scientific, 1990.

JOURNALS

Journal of Electrochemistry
Journal of Surface science
Journal of Physical Chemistry (A, B and C)
Langmuir
Statistical Thermodynamics

WEB RESOURCES

http://www.acs.org/content/acs/en/careers/college-to-career/areas-of-chemistry/physical-chemistry.html
http://www.annualreviews.org/journal/physchem

PATTERN OF EVALUATION

CONTINUOUS ASSESSMENT:

Total Marks:50 **Duration: 90 mins.**

Section A – 11 x 1 = 11 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match and answer in a line or two)
Section B – 3 x 8 = 24 Marks (3 out of 4 to be answered)
Section C – 1 x 15 = 15 Marks (1 out of 2 to be answered)

Third Component:
List of evaluation modes:
Quiz
Problem Solving
Seminars
Assignments

END SEMESTER EXAMINATION:

Total Marks: 100 **Duration: 3 hours**

QUESTION PAPER PATTERN

Section A – 20 x 1 = 20 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match and answer in a line or two)
Section B – 5 x 8 = 40 Marks (5 out of 7 to be answered)
Section C – 2 x 20 = 40 Marks (2 out of 3 to be answered)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086
M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS
(Effective from the academic year 2015 – 2016)

STRUCTURAL INORGANIC CHEMISTRY

CODE: 15CH/PC/SI14 **CREDITS: 4**
L T P: 4 1 0
TOTAL TEACHING HOURS: 65

OBJECTIVES OF THE COURSE

- To provide knowledge required to appreciate and analyse the chemistry of structurally important compounds
- To give an overview and understanding of transition metal compounds and organometallic compounds
- To provide fundamental knowledge about industrially important non-transition metal compounds

Unit 1

Structure and Defects in Solids (14 hrs.)

1.1 Lattice Energy, Born Lande Equation, Packing of Ions in Crystals, % Void, Crystal Imperfections – Stoichiometric Defects (Schottky, Frenkel) and Non-Stoichoiometric Defects (F Center), Problems related to Defects, Conductivity by Ion Migration, Factors Affecting Crystal Structures

1.2 Structures of Simple Inorganic Solids of Type AX, AX_2, A_2X_3, Perovskite, Spinel and Inverse Spinels

1.3 Bonding in Metals: Band Theory and Metallic Properties. Interstitial Compounds, Insulators, Semi Conductors and Super Conductors. Super Conductivity-Principle, Meissner Effect

1.4 Electrical Properties of Solids- Dielectric, Ferroelectric, Pyroelectric and Piezoelectric Properties and Relation between Pyro, Piezo and Ferroelectric Properties. Magnetic Properties of Solids-Curie-Weiss Law

Unit 2

Techniques of Structure Determination in Solid State (8 hrs.)

2.1 X-Ray Diffraction Studies - Structural Determination of NaCl using Powder Method.

2.2 Electron and Neutron Diffraction Studies- Principles and Applications

Unit 3

Structure and Chemistry of Organometallic Compounds (18 hrs.)

3.1 Classification of Organometallic Compounds

3.2 Preparation, Bonding and Structure of Metal Carbonyls, Metal Nitrosyls (Application of EAN Rule and 18-Electron Rule) and Metal Hydride Complexes. Alkyl Complexes, Carbenes, Carbynes, Carbides, Non Aromatic Alkene and Alkynecomplexes, Allyl and Pentadienyl Complexes, Aryl Complexes, Carbonyl Hydride Complexes, Triphenyl Phosphine and Dinitrogen Complexes

3.3 Application of IR Spectroscopic Technique to the Study of the Structure of Metal Carbonyls and Nitrosyls

3.4 Molecular Orbital Treatment of Metallocenes -Ferrocene

Unit 4

Organometallic Compounds in Catalysis (12 hrs.)

4.1 Olefins-Wilkinson's Catalyst, Oxo Process, Ziegler- Natta Catalysis, Wacker Process, Cyclo-oligomerisation (Reppe's Catalyst).

4.2 Role of Catalyst in Monsanto Acetic Acid Process and in the Synthesis of Gasoline

Unit 5

Structure and Chemistry of Non- transition and Transition Metals (13 hrs.)

5.1 Preparation, Properties and Structures of Boranes (Wades Rules), Phophazenes, Carboranes, Metallocarboranes, Silicates and Silicones, Supramolecular Assembly-Zeolites.

5.2 Preparation, Properties and Structures of iso and heteropolyacids of Mo and W.

TEXTBOOKS

Cotton, F.A. and Wilkinson G. *Advanced Inorganic Chemistry*, New York : John Wiley, 2000.

Huheey, James E. and Keiter. Ellen A. *Inorganic Chemistry - Principles of Structure and Reactivity,* New York :Addison Wesley , 2004.

BOOKS FOR REFERENCE

Atkins ,Peter, Fraser Armstrong, Jonathan Rourke, Mark Weller and Tina Overton, *Inorganic Chemistry*, Oxford: Oxford Press, 2010

Jolly, W.L. Modern *Inorganic Chemistry*, New York : McGraw Hill,1994.

Moeller, T. *Inorganic Chemistry*, New York: John Wiley, 1982.

Purcell Keith, F. and John C. Kotz, *An Introduction to Inorganic Chemistry,* Philadelphia :W.B.Saunders Company, 1982.

Wells, A.F. *Structural Inorganic Chemistry*, London: ELBS, 1981.

West, A.R. *Solid State Chemistry and its Applications*, New York: John Wiley, 2014.

JOURNALS

Journal of Inorganic Chemistry

Journal of Organometallic Chemistry

International Journal of Inorganic Chemistry

Inorganic Chemistry Frontiers

WEB RESOURCES

http://www.chem.iitb.ac.in/~rmv/ch102/ic6.pdf
https://www2.chemistry.msu.edu/faculty/reusch/virttxtjml/orgmetal.htm
http://www.tandfonline.com/toc/gcic20/current#.VQL8TnyUflg
http://www.sciencedirect.com/science/bookseries/08988838

PATTERN OF EVALUATION

CONTINUOUS ASSESSMENT:

Total Marks: 50 **Duration: 90 mins.**

Section A – 11 x 1 = 11 Marks
(All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)
Section B – 3 x 8 = 24 Marks (3 out of 4 to be answered)
Section C – 1 x 15 = 15 Marks (1 out of 2 to be answered)
Third Component:
List of evaluation modes:
Quiz
Seminars
Assignments

END SEMESTER EXAMINATION:

Total Marks: 100 **Duration: 3 hours**

Section A – 20 x 1 = 20 Marks
(All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)
Section B – 5 x 8 = 40 Marks (5 out of 7 to be answered)
Section C – 2 x 20 = 40 Marks (2 out of 3 to be answered)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086
M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS
(Effective from the academic year 2015 – 2016)

PHYSICAL CHEMISTRY – PRACTICAL

CODE: 15CH/PC/P112 **CREDITS : 2**
L T P: 0 0 3
TOTAL HOURS: 39

Unit 1
Phase Rule

Three Component System (Water-Toluene- Acetic Acid)

Unit 2
Solubility Product

Variation of the Solubility of (Calcium Sulphate /Zinc Sulphate/ Nickel Sulphate) with Ionic Strength and Determination of the Thermodynamic Solubility Product (Complexometric Titration with EDTA)

Unit 3
Chemical Kinetics

1. Effect of Ionic Strength on the Reaction Rate: Persulphate and Potassium Iodide Reaction
2. Kinetics of Hydrolysis of t-Butyl Chloride (by Conductometric Measurements)

Unit 4
Viscometry

Determination of Relative Molecular Mass / Intrinsic Viscosity of Polystyrene from Viscosity Measurements

Unit 5
Partial Molal Quantities

Determination of Partial Molal Volume of Methanol in Dilute Aqueous Solutions (by Method of Intercepts)

Unit 6
Conductometry

1. Determination of Critical Micelle Concentration Conductometrically.
2. Titration of Mixture of Three Acid (Trichloroacetic Acid, Dichloroacetic Acid and Acetic Acid) Conductometrically

Unit 7
pH metry

Determination of pKa Values of Glycine /Malonic Acid / Phosphoric Acid Potentiometrically using Glass Electrode

BOOKS FOR REFERENCE

Viswanathan, B. and Raghavan, P.S. *Practical Physical Chemistry*. New Delhi :Viva Books, 2005.

Venkateswaran, V. Veerasamy, R. Kulandaivelu, A. R. *Principles of Practical Chemistry*. New Delhi : Sultan Chand , 1997.

Findlay, Alexander, *Practical Physical Chemistry*. London: Longman Green, 1973.

END SEMESTER EXAMINATION :

Total Marks: 50 **Duration : 3 hours**

Procedure = 10 (marks)
Vivavoce = 10 (marks)
Reported value = 30 (marks)

CONTINUOUS ASSESSMENT (INTERNAL):

Total Marks : 50

Class Work = 30 (marks) – inclusive of *viva*
CA Test = 20 (marks)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086
M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS
(Effective from the academic year 2015 – 2016)

INORGANIC QUALITATIVE AND QUANTITATIVE ANALYSIS - PRACTICAL

CODE :15CH/PC/P214 **CREDITS: 4**
L T P: 0 0 6
TOTAL HOURS: 78

Unit 1

Semimicro Qualitative Analysis

Analysis of four cations- two rare cations and two common cations- in a salt mixture.

Unit 2

Quantitative Analysis

Complexometry : Estimation of Mg^{2+}, Zn^{2+}, Ca^{2+} and Ni^{2+}

Cerimetry : Estimation of Fe^{2+} / Oxalic acid

Determination of Chlorine in bleaching powder.

Unit 3

Preparation of Inorganic Complexes

Tetraammine copper (II) sulphate
Tris (thiourea) copper (I) sulphate
Hexaammine cobalt (III) chloride
Bis (acetylacetanato) copper (II) / Bis (acetylacetanato) nickel (II)

A comprehensive viva will be conducted during the practical hours

BOOKS FOR REFERENCE

Ramanujam, V.V. *Inorganic Semimicro Qualitative Analysis***.** Chennai: National, 1995.

Mendham J., Denny R.C., Barnes J.D and Thomas M. *Vogel's Text Book of Quantitative Chemical Analysis*, London: Pearson Education, 2002.

END SEMESTER EXAMINATION

Total Marks : 100 **Duration: 6 hours**

Inorganic complex preparation : **10 Marks**
Preparation – quantity & quality [10]

Semi micro qualitative analysis : **40 Marks**
General Procedure- 10 Marks Rare radicals (2 X 10) -20 Marks
Common radicals – (2 X 5) - 10 Marks

Volumetric Analysis : **40 Marks**

Error 1% = 40 Marks
2% = 35 Marks
3% = 25 Marks
Viva : **10 marks**

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086
M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS
(Effective from the academic year 2015 – 2016)

ORGANIC CHEMISTRY-II

CODE: 15CH/PC/OC24 **CREDITS : 4**
L T P : 4 1 0
TOTAL TEACHING HOURS : 65

OBJECTIVES OF THE COURSE

- To understand the importance of reaction intermediates
- To suggest mechanisms for a given reaction.
- To understand the application of photochemistry and concerted reactions in the field of organic chemistry.

Unit 1

Reactive Intermediates **(14 hrs.)**

1.1 Formation, Stability, Reactions and Rearrangements
- Carbocations (Wagner Meerwein Rearrangements)
- Carbanions (Wittig, Favorski Rearrangement)
- Carbene(Skattebol , Wolff Rearrangement, Insertion of C-H and X-H bonds),
- Nitrenes (Hofmann, Schmidt, Lossen, Curtius, Beckmann rearrangements),
- Carbon Radicals (Acyloin Condensation,Dimerisation, McMurry Reactions)
- Arynes (Dimerisation Reactions)

1.2 Neighbouring Group Participation and Non-classical Carbonium ion.

Unit 2

Condensation, Addition, Elimination and Substitution Type Name Reactions (14 hrs.)

2.1 Condensation- Aldol, Perkin, Stobbe, Dieckmann, Claisen , Mannich

2.2 Addition-Grignard, Diels-Alder, Michael, Hydroboration, Robinson, Annulation, Woodward and Prevost Hydroxylation, Reformatsky, Stork enamine reactions

2.3 Substitution- Chichibabin, Friedel-Crafts, Vilsmeier-Haack, Reimer-Tiemann,

2.4 Gatterman-Koch, Hoesch, Bischler-Napieralski, Hunsdiecker, Fries, Sommelet- Hauser rearrangements

2.5 Elimination- Peterson synthesis, Shapiro, Cope

Unit 3

Oxidation and Reduction Reactions **(10 hrs.)**

3.1 Reduction- Birch, Wolff Kishner, Clemmenson and selective reduction of 4-tert-butyl cyclohexanone using selective-hydride reduction

3.2 Oxidation- Oppenaeur, Swern, Baeyer Villiger, SeO_2 (methylene to carbonyl), Allylic Oxidation of Olefins, Cr(VI) reagents, Oxidation of Aryl Methanes

Unit 4

Photochemistry **(10 hrs.)**

4.1 Fundamentals of Photochemistry, Jablonski Diagram

4.2 Cis-trans Isomerisation, Paterno Buchi Reaction ,Norrish type-I and type- II Reactions, di-pi methane Rearrangement.

4.3 Photochemistry of Cyclohexadienones

4.4 Photoreduction of ketones and Photooxidation of olefins.

Unit 5

Pericyclic Reactions (17 hrs.)

5.1 Classification, Orbital Symmetry, Woodward- Hofmann Rules (con & dis rotation).

5.2 Electrocyclic Reactions-Thermal and Photochemical (cyclisation and ring openings). Stereochemistry, FMO and Correlation Diagrams for butadiene to cyclobutene and 1, 3, 5-hexatriene to 1, 3- cyclohexadiene systems.

5.3 Cycloaddition Reactions- Thermal and Photochemical, Stereochemistry, FMO and Correlation Diagrams of (2+2 and 4+2) Reactions.

5.4 Sigmatropic rearrangements – Cope, oxy-Cope and Claisen rearrangement.

5.5 Cheletropic Reactions

5.6 Fluxional Molecules – Homotropylidene, barbaelone, bullvalene.

TEXT BOOKS

Ahuliwalia, V.K. and R.K .Parashar. *Organic Reaction Mechanism***.** New Delhi: Narosa, 2002.

Bruckner, R.*Advanced Organic Chemistry: Reaction Mechanisms*.USA: Academic Press, 2003.

Singh, Jagadamba, Jaya Singh. *Photochemistry and Pericyclic Reactions*. New Delhi: New Age, 2005.

March, Jerry. *Advanced Organic Chemistry*.New York: Wiley,2007.

BOOKS FOR REFERENCE

Jonathan Clayden, Nick Greeves, Stuart Warren, *Organic Chemistry*.New York: Oxford University Press, 2012.

Carey, A. Francis, Richard J. Sundberg, *Advanced Organic Chemistry Part A: Structure and Mechanisms*. New York: Springer, 2007.

Carruthers, W.and I. Coldham, *Modern Methods of Organic Synthesis.*UK:Cambridge University Press, 2005.

Turro, N.J. *Modern Molecular Photochemistry*. Sausalito: University Science Books, 1991.

Solomons, T.W Graham and Craig B. Fryhle, *Organic Chemistry*. New York: John Wiley, 2000.

Moody, C.J. and Witham G.H. *Organic Reactive Intermediates***.** New York: Oxford Chemistry, 1992.

Bansal, K. Raj, *Organic Reaction Mechanism*. New Delhi:Tata McGraw-Hill, 2006.

JOURNALS

Topics in Current Chemistry

Angewandte Chemie

Acta Chemica Scandinavica

Pure and Applied Chemistry

WEB RESOURCES

http://www.grc.org/programs.aspx?id=11812

www.ijrpbsonline.com

PATTERN OF EVALUATION

CONTINUOUS ASSESSMENT:

Total Marks: 50 **Duration: 90 mins.**

Section A – 11 x 1 = 11 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

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Section C – 1 x 15 = 15 Marks(1 out of 2 to be answered)

Third Component Tests:

List of evaluation modes:
Quiz
Seminars
Assignments

END SEMESTER EXAMINATION:

Total Marks: 100 **Duration: 3 hours**

Section A – 20 x 1 = 20 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 5 x 8 = 40 Marks (5 out of 7 to be answered)

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M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

QUANTUM CHEMISTRY AND GROUP THEORY

CODE: 15CH/PC/QG24 **CREDITS: 4**

L T P: 4 1 0

TOTAL TEACHING HOURS: 65

OBJECTIVES OF THE COURSE

- To give an understanding of basic principles of quantum mechanics and their applicability to study the internal structure of atoms and molecules
- To enable an understanding of the important concepts of group theory

Unit 1

Matter Waves and Quantum Mechanical Formalism **(10 hrs.)**

1.1 Wave Particle Duality, Uncertainty Principle, Particle Wave and Schrödinger Wave Equation, Wave Functions, Properties of Wave Function. Conditions of Normalization and Orthogonality

1.2 Operators and their Algebra, *Eigen* Values and *Eigen* Functions, Hermitian Properties of Operators, Postulates of Quantum and some Theorems Related the same

1.3 Free Particle, Particle in One Dimensional Box with Infinite Potential Barrier, Quantization and Quantum Numbers, Use of Box Model, Particle in a Three Dimensional Box, Degeneracy, Particle in a Box with Finite Potential Barriers, Quantum Mechanical Tunneling, Problems

Unit 2

Application to Simple Systems **(16 hrs.)**

2.1 Harmonic Oscillator (Classical & Quantum Mechanical), Schrodinger Wave Equation and Its Solution, Hermite Polynomial, Complete Wave Function, Vibrational Quantum Numbers, Physical Picture of Ψ and Ψ^2.

2.2 Particle in a Sphere, Schrödinger Wave Equation in Spherical Coordinates(Derivation Not Expected), Legendre and Associated Legendre Functions, Rotational Quantum Numbers, Spherical Harmonics, Rotation of a Diatomic Molecule, Problems

2.3 Schrodinger Wave Equation in Spherical Coordinates, Splitting Equation into R, Θ and Φ Equations, Solving R-Equation, Laguerre Polynomial and Associated Laguerre Polynomials, Radial Functions, Quantum Numbers n and l, Energy Eigenvalues in Atomic Units, Complete Wave Function of Hydrogen Like Atoms, Physical Representation of Orbitals, Radial Plots and Angular Plots, Probability Function and Plots, Average Distance of Electron, Problems

2.4 Approximation Methods – Variational Method (Linear Band Non-Linear Variation), Perturbation Theory (Non-Degenerate, First Order), Application to Helium Atom. Ground State

Unit 3

Atomic Structure **(16 hrs.)**

3.1 Symmetric and Anti Symmetric Wave Functions, Electron Spin, Spin Orbitals, Pauli's Principle

3.2 Excited State of He Atom, Singlet and Triplet States.

3.3 Hartee- Fork Self Consistent Field Theory. Walsh Diagrams. Angular Momentum of many Electron Atoms, Ladder Operators

3.4 LCAO-MO for H_2^+, Molecular Orbital Approximation for Ethylene, Butadiene and Benzene. Plots and Nodes of Molecular Orbitals

Unit 4

Group theory: Fundamental Concepts (16 hrs.)

4.1 Symmetry Operation and Elements, Defining Coordinate System, Combining Symmetry Operations, Symmetry Point Groups, Point Group of Molecules, Systematic Point Group Classification, Optical Activity and Symmetry

4.2 Irreducible Representation, Unit Vector Transformation, Reducible Representations, Systematic Reduction of Reducible Representation

4.3 Group Multiplication Tables, Sub Groups and Classes, the Great Orthogonality Theorem

4.4 Construction of Character Table for Point Groups. ($D_{2h,}$ C_{2V}, C_{3V}), Explanation for the Complete Character Table for the above Groups

Unit 5

Application of group theory (7 hrs.)

5.1 Application of Group Theory in (I) Electronic Spectra –HCHO (Ii) Vibrational Spectra –H_2O

5.2 Application of Group Theory in Hybridization Schemes for Simple Molecules-CH_4, H_2O, NH_3

TEXTBOOKS

Prasad, R.K. *Quantum Chemistry*. New Delhi: New Age International, 1997.

Atkins, P.W. *Molecular Quantum Mechanics*. Oxford: Clarendon Press, 2006.

Chandra, A.K. *Introductory Quantum Chemistry*. New Delhi: Tata McGraw- Hill, 2006.

Cotton, F.A.*Chemical Applications of Group Theory*. New Delhi :Wiley Eastern, 2000.

BOOKS FOR REFERENCE

Carter, R.L.*Molecular Symmetry and Group Theory*. New Delhi: John Wiley, 2005.

Levine, I.R.*Quantum Chemistry*. New Delhi: Prentice Hall of India, 1994.

Prasad, R.K. *Quantum Chemistry through Problems and Solutions*. New Delhi: New Age International, 1997.

Lowe, J.P.*Quantum Chemistry*. SanDiego: Academic Press, 1993.

McQuarrie, A.Donald, *Quantum Chemistry***.** Oxford: Oxford University Press, 1982.

Cox, P.A. *Introduction to Quantum Theory and Atomic Structure,* Oxford: Oxford University Press, 1996.

Albright, T.A. and J.K.Burdett, *Problems in Molecular Orbital Theory*, Oxford: Oxford University Press, 1992.

Bishop, D.M. *Group Theory and Chemistry*. New York: Dover, 1993.

JOURNALS

International Journal of Quantum Chemistry
Langmuir
Journal of Group Theory

WEB RESOURCES

http://symmetry.otterbein.edu/gallery/
http://ctg.epfl.ch/

PATTERN OF EVALUATION

CONTINUOUS ASSESSMENT:

Total Marks: 50 **Duration: 90 mins.**

Section A – 11 x 1 = 11 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 3 x 8 = 24 Marks (3 out of 4 to be answered)

Section C – 1 x 15 = 15 Marks (1 out of 2 to be answered)

Third Component Tests:

List of evaluation modes:
Quiz
Seminars
Assignments

END SEMESTER EXAMINATION:

Total Marks: 100 **Duration: 3 hours**

Section A – 20 x 1 = 20 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 5 x 8 = 40 Marks (5 out of 7 to be answered)

Section C – 2 x 20 = 40 Marks (2 out of 3 to be answered)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086

M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

COORDINATION CHEMISTRY

CODE: 15CH/PC/CO24 **CREDITS: 4**

L T P: 4 1 0

TOTAL TEACHING HOURS: 65

OBJECTIVES OF THE COURSE

- To enable the students to gain an understanding of the principles of bonding in coordination complexes
- To enable the students to appreciate the importance of electronic spectra and magnetic properties of complexes
- To provide an insight into the biological role of metal ions in everyday life

Unit 1

Introduction to Coordination Complexes (15 hrs.)

1.1 Nomenclature, Stereochemistry and Isomerism of Complexes With Coordination Number 2 to 6, Stability of Complexes, Thermodynamic Aspects, Successive and Overall Formation Constants –Factors affecting Stability of Complexes -Chelate Effect - Importance of Chelates and Determination of Stability Constants

1.2 Theories of Bonding in Complexes: Valence Bond Theory, Crystal Field Theory- Crystal Field Splitting in O_h, T_d, Tetragonal and Square planar Complexes. Factors Influencing Magnitude of Δ_O – Spectrochemical Series, CFSE and Applications of CFT. Distortion in O_h Complexes - Jahn Teller Effect

1.3 Ligand Field Theory and Molecular Orbital Theory – Qualitative Treatment of LCAO Method, MO Energy Diagrams of Sigma and Pi Bonding in O_h Complexes

Unit 2

Spectral Characteristics of Metal Complexes (18 hrs.)

2.1 Types of Absorption Spectra, Spectral Terms – Russell-Saunders States, Electronic States – Terms Resulting From d^n Configuration, Selection Rules

2.2 Correlation Diagrams – Orgel and Tanabe-Sugano Diagrams, Racah Parameters and Nephelauxetic Series, Electronic Spectra of d^{1-9} Metal Complexes. Charge Transfer Spectra

2.3 Electronic Spectra of Lanthanide & Actinide Complexes

2.4 Mössbauer Spectra of Iron and Tin Complexes

2.5 ESR Spectra of Copper and Cobalt Complexes

Unit 3

Magnetic Characteristics of Complexes (8 hrs.)

3.1 Types of Magnetic Properties, Magnetic Properties of Complex Ions – Lanthanides & Actinides

3.2 Orbital Contribution to Magnetic Moment, Quenching of Orbital Angular Moment, Spin-Orbit Coupling

Unit 4

Reaction Mechanisms in Complexes (15 hrs.)

4.1 Kinetics and Mechanisms of Reactions of Complexes: Substitution Reactions of $O_h$complexes - Mechanism of Water Replacement - Acid Hydrolysis and Basehydrolysis - S_N1CB Mechanism

4.2General Mechanism of Square Planar Substitution Reactions: Two Parallel Pathways - Factors Affecting the Reactivity of Square Planar Complexes of d^8metal Ions - Trans Effect - Theories of Trans Effect

4.3 Mechanism of Electron Transfer Reactions: Outer Sphere Electron Transfer Reactions - Marcus Theory and Inner Sphere Electron Transfer Reactions-Formation and Rearrangement, Nature of the Bridge Ligand in Inner Sphere Electron Transfer Reactions. Non-Complementary Reactions

4.4 Photochemical Reactions of Transition Metal Complexes: Photosubstitution and Photo isomerisation of Cobalt and Chromium Complexes

Unit 5

Bio-Inorganic Chemistry (9 hrs.)

5.1 Biological Importance of Trace Elements

5.2 Structure and Functions of Metalloporphyrins:

-Transport and Storage of Oxygen (Haemoglobin and Myoglobin)

- Electron Transfer- Cytochromes

- Vitamin B_{12} (Cyanocobalamin)

-Photosynthesis (Chlorophyll)

5.3 Iron Storage - Ruberedoxins and Ferredoxins

5.4 Biological Redox Systems- Plastocyanin

TEXTBOOKS

Cotton, F.A. and G.Wilkinson, *Advanced Inorganic Chemistry*. New York: John Wiley, 2000.

Huheey, E. James and Ellen A. Keiter, *Inorganic Chemistry - Principles of Structure and Reactivity*. New York: Addison Wesley 2004.

BOOKS FOR REFERENCE

Jolly, W.L. *Modern Inorganic Chemistry*. New York: McGraw – Hill, 1991.

Moeller, T. *Inorganic Chemistry*. New York: John Wiley, 1990.

Purcell, Keith.F. and John C.Kotz. *An Introduction to Inorganic Chemistry***,** Philadelphia: W.B.Saunders, 1982.

Wells, A.F. *Structural Inorganic Chemistry*. London: ELBS,1981.

JOURNALS

Journal of Inorganic Chemistry

Journal of Coordination Chemistry

WEB RESOURCES

http://www.chemistry.wustl.edu/~edudev/LabTutorials/naming_coord_comp.html

http://chemed.chem.purdue.edu/genchem/topicreview/bp/ch12/names.php

PATTERN OF EVALUATION

CONTINUOUS ASSESSMENT:

Total Marks: 50 **Duration: 90 mins.**

Section A – 11 x 1 = 11 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 3 x 8 = 24 Marks (3 out of 4 to be answered)

Section C – 1 x 15 = 15 Marks (1 out of 2 to be answered)

Third Component Tests:

List of evaluation modes:
Quiz
Seminars
Assignments

END SEMESTER EXAMINATION:

Total Marks: 100 **Duration: 3 hours**

Section A – 20 x 1 = 20 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 5 x 8 = 40 Marks (5 out of 7 to be answered)

Section C – 2 x 20 = 40 Marks (2 out of 3 to be answered)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086

M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

ORGANIC SEPARATION AND ANALYSIS - PRACTICAL

CODE: 15CH/PC/P324 **CREDITS : 4**

L T P : 0 0 6

TOTAL HOURS: 78

Unit 1

Preparation of Reagents used for Qualitative Organic Analysis

Tollen's reagent, Fehling's Reagents A & B, Barfoed's reagent, Benedict's Reagent, Molisch's reagent, Bromine Water, Brady's reagent, Schiff's reagent

Unit 2

Separation and analysis of a mixture of two organic compounds

- Solvent separation based on solubility in acid, base or neutral media
- Pilot separation & Bulk separation
- Identification of functional groups, Preparation of derivatives for functional groups and determination of their melting points
- Compounds can be separated using Soxhlet and Rotary Vaccum Evaporator (demonstration only)
- Identification of separated compounds & derivatives using UV and IR(demonstration only)

A comprehensive viva will be conducted during the practical hours

BOOKS FOR REFERENCE

Ahluwalia,V.K. and Renu Agarwal. *Comprehensive Practical Organic Chemistry-Preparation and Quantitative Analysis*. Hyderabad: University Press, 2000.

Mohan, J. *Organic Analytical Chemistry–Theory and Practice***.** New Delhi: Narosa, 2003.

Bansal, K.Raj. *Laboratory Manual of Organic Chemistry***.** New Delhi: Wiley Eastern, 1994.

Vogel, A.I. *Elementary Practical Organic Chemistry Part II, Qualitative Organic Analysis***.** New Delhi: CBS Publishers, 1998.

Unit 1 to be tested internally

PATTERN OF EVALUATION

END SEMESTER EXAMINATION:

Total Marks : 50 **Duration : 6 hours**

Pilot test		: 4 marks
For each compound:		
Aliphatic/Aromatic	: 1 mark	
Saturated/Unsaturated	: 1 mark	
Special Elements	: 3 marks	
Procedure	: 4 marks	
Derivative	: 2 marks	
Functional Group	: 4+2 marks	
Melting point	: 1 mark	
Total	: 18 marks	
For two compounds	: 2 x 18	: 36 marks
Viva voce		: 10 marks
TOTAL		**: 50 marks**

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086

M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

SYNTHETIC ORGANIC CHEMISTRY AND NATURAL PRODUCTS

CODE: 15CH/PC/SO34 **CREDITS: 4**

L T P: 4 1 0

TOTAL TEACHING HOURS: 65

OBJECTIVES OF THE COURSE

- To perform retrosynthetic analysis and identify the target molecule
- To design synthesis of a given compound
- To appreciate the role of reagents in the synthesis of organic compounds
- To impart knowledge on the extraction and synthesis of natural products

Unit 1

Strategies for Synthesis **(15 hrs.)**

1.1 Definitions, Synthons and Synthetic Equivalents, Guidelines, Functional Group Interconversion and Planning for Synthesis of Organic Compounds

1.2 Disconnection Approach – One Group C-X, Two Group C-X, One Group C-C and Two Group C-C Disconnections

1.3 Chemoselectivity, Reversal Polarity (Umpolung) and Ammine Synthesis

1.4 Protection and Deprotection – Alcohols, Carbonyls, Carboxylic Acids and Amino Functional Groups

1.5 Retrosynthetic Analysis- Alternate Synthetic Routes. Synthesis of Organic Mono and Bifunctional Compounds Via Disconnection Approach

1.6 Stereochemical Control of Products-Selective Aldol and Michael Reactions

Unit 2

Novel Reagents in Organic Synthesis **(16 hrs.)**

Use of the Following Reagents in Organic Synthesis and Functional Group Transformations:

2.1 Diborane, OsO_4, NBS, Phenylisothiocyanate, DCC, Lead Tetraacetate, PCC, Tosyl Chloride, Trifluoroacetic Acid, DDQ, Selenium Dioxide, TMSI and Dithianes, Perbenzoic Acid

2.2 Bakers Yeast

Unit 3 **(12 hrs.)**

Organometallic Reagents in Organic Synthesis

Organometallic Reagents- Crown Ether Complexes, n-Butyl Lithium, LDA, LAH, tri-n-Butyl Tin Hydride, Aluminium, Silicon, Copper, Cobalt, Zinc and Palladium Compounds

Unit 4

Alkaloids, Terpenoids and Steroids **(12 hrs.)**

4.1 General Methods of Structure Determination of Alkaloids, Terpenoids and Steroids

4.2 Structure Elucidation of Zingiberine (Terpenoid), Papaverine and Reserpine (Alkaloids)

4.3 Constitution of Cholesterol – Structure of the Nucleus, Position of the Hydroxyl Group and Double Bond, nature and position of the side-chain, position of the angular Methyl Group

Unit 5

Natural Pigments **(10 hrs.)**

5.1 Anthocyanins – Introduction, Isolation, Determination of Structure of Anthocyanins and General Methods for the Synthesis of Anthocyanidins

5.2 Flavones and Flavonols: Introduction, Isolation, General Properties, Basic Structure of Flavones and Flavonols, General Methods for Determination of the Structure of Flavones Taking Flavone as an Example

5.3 Structure Elucidation of Apigenin (Flavones), Quercetin (Flavonols) and Daidzein (Isoflavones)

5.4 Distinction of Flavonoids by Characteristic Colour Reactions and Absorption Spectra (UV-Visible)

TEXT BOOKS

Warren,Stuart. S. *Organic Synthesis- the Disconnection Approach.* New York: Wiley, 2013.

Sanyal, S.N. *Reactions, Rearrangements and Reagents*. New Delhi: Bharathi Bhawan , 2006.

Singh, Jagadamba and L.D.S .Yadav.*Advanced Organic Chemistry*. Meerut: Pragati Prakashan, 2010.

Singh, J, S.M.Ali and Jaya Singh. *Natural Produts Chemistry.* Meerut: Pragati Prakashan, 2010.

BOOKS FOR REFERENCE

Jonathan, Clayden, Nick Greeves, Stuart Warren. *Organic Chemistry*. New York: Oxford University Press, 2012.

Carey , A.Francis and Richard J. Sundburg. *Advanced Organic Chemistry Part B: Reactions and Synthesis***.** New York : Springer, 2007.

Harmata, Michael .*Strategies and Tactics in Organic Synthesis*. London: Academic Press, 2008.

Norman, R.O.C and J.M.Coxon.*Principles of Organic Synthesis*. New York: CRC Press, 2012.

Bhat, V. Sujata , Bhimsa A. Nagasampagi, Meenakshi SivaKumar. *Chemistry of Natural Products* , India : Narosa, 2005.

Finar, I.L. *Organic Chemistry*. London : ELBS, 2000.

Agarwal, O.P. *Chemistry of Organic Natural Products.* Meerut: Krishnan Prakasan, 2010.

JOURNALS

Journal of the American Chemical Society
The Journal of Organic Chemistry
Tetrahedron Letters
Journal of Natural Products

WEB RESOURCES

www.oxfordtextbooks.co.uk/orc/clayden2e/

http://pubs.acs.org/doi/abs/10.1021/jm500941m

PATTERN OF EVALUATION

CONTINUOUS ASSESSMENT:

Total Marks: 50 **Duration: 90 mins.**

Section A – 11 x 1 = 11 Marks(All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 3 x 8 = 24 Marks (3 out of 4 to be answered)

Section C – 1 x 15 = 15 Marks (1 out of 2 to be answered)

Third Component Tests:

List of evaluation modes:
Quiz
Seminars
Assignments

END SEMESTER EXAMINATION:

Total Marks: 100 **Duration: 3 hours**

Section A – 20 x 1 = 20 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 5 x 8 = 40 Marks(5 out of 7 to be answered)

Section C – 2 x 20 = 40 Marks(2 out of 3 to be answered)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086

M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

MOLECULAR SPECTROSCOPY

CODE: 15CH/PC/MS34 **CREDITS: 4**

L T P: 4 1 0

TOTAL TEACHING HOURS: 65

OBJECTIVES OF THE COURSE

- To understand the principles of various spectroscopic techniques
- To interpret the spectra of molecules and predict the structure of compounds
- To understand the complementary nature of spectra in structural elucidation

Unit 1

Rotational, Vibrational, Rotational-vibrational Spectroscopy (17 hrs.)

1.1 Rotational Spectroscopy: Classification of Rotors Based on Moment of Inertia, Diatomic Molecules as Rigid Rotors and Non-Rigid Rotors - Rotational Energy Levels, Transitions, Selection Rules and Effect of Isotopic Substitutions. Inversion Phenomena and Stark Effect. Rotational Spectra of Linear, Symmetric and Asymmetric Top Polyatomic Molecules

1.2 Vibrational Spectroscopy : Diatomic Molecules as Harmonic and Anharmonic Oscillators – Energy Levels and the Vibrational Transitions. Vibrations of Polyatomic Molecules – Fundamental Vibrations, Overtones, Combination Bands and Symmetry of Linear and Nonlinear Molecules

1.3 Vibrational - Rotational Spectroscopy- Diatomic Vibrating Rotator- Energy Levels, Transitions, and Selection Rules. Parallel and Perpendicular Vibrations of Linear Poly Atomic Molecules and Symmetric Top Molecules. Effect of Nuclear Spin. Raman Spectroscopy- Raman Effect, Rule of Mutual Exclusion and Resonance Raman Effect. Raman as Complementary to IR. Structure Determination of CO_2, N_2O,SO_2, NO_3^-, ClO_3^- and ClF_3

1.4 Interpretation of IR Spectra: Group Frequencies of various Functional Groups. Factors affecting Group Frequencies

Unit 2

Electronic Absorption Spectroscopy (10 hrs.)

2.1 Principle of UV-Visible Spectroscopy, Electronic Spectra of Diatomic Molecules - Born – Oppenheimer Approximation, Franck Condon Principle, Dissociation and Predissociation Energy

2.2 Molecular Term Symbols (Diatomic Molecules)

2.3 Characterization of Organic Compounds: Factors Affecting Absorption Spectra. Application of Woodward-Fieser Rules to Conjugated Dienes, α,β- Unsaturated Carbonyl Compounds, Benzene and its Substituted Derivatives and Polycyclic Aromatic Hydrocarbons. Fieser-Kuhun Equation – Study of Polyene Systems

Unit 3

Nuclear Magnetic Resonance Spectroscopy (15 hrs.)

3.1 NMR Phenomena, Nuclear Spin, Bloch Equations and Types of Relaxation Processes

3.2 Parameters of ^{1}H-NMR: Chemical Shift, Shielding and Deshielding, Factors affecting δ. Chemical Structure Correlations of δ, Chemical and Magnetic Equivalence of Spins

3.3 ^{1}H-NMR: Spin-Spin Splitting, Application of Spin-Spin Splitting to Structure Determination. Effect of Coupling Constants –Geminal Coupling, Viccinal Coupling and Long Range Coupling

3.4 ^{13}C-NMR :Comparison of ^{13}C and ^{1}H-NMR, Spin Decoupling , The Nuclear Overhauser Effect , Peak Intensity, Chemical Classes, Chemical Shifts, ^{13}C-^{1}H and ^{13}C-^{13}C Spin Coupling - DEPT. Structure Determination of Simple Aliphatic and Aromatic Compounds

3.5 An Introduction to NMR in Solid State, FID, 2D and 3D NMR. ^{15}N, ^{31}P and ^{19}F NMR – Spectra of Simple Inorganic Compounds

Unit 4

Mass Spectrometry (17 hrs.)

4.1 Basic Principles, Fragmentation Types and Rules. Interpretation of Mass Spectra- Molecular Ion Peak, Isotope Peaks, Base Peak, Metastable Peak, Nitrogen Rule. Calculation of Isotopic Distributions – Carbon and Halogen Isotopes using Binomial Expressions

4.2 Fragmentation Patterns: Cleavage of Sigma Bond- Even Electron Rule, α- Cleavage- Stevenson's Rule, Benzylic Bond Cleavage, Inductive Cleavage, Retro Diels-Alder Cleavage and Mclafferty Rearrangement

4.3 Structure Determination of Organic Compounds and Inorganic Compounds - Metal Halide Salts and Coordination Complexes

Unit 5 (6 hrs.)

Determination of structure of organic and inorganic compounds by comprehensive (UV, IR, NMR and Mass) spectral data

TEXT BOOKS

Banwell, Colin and Mckash Elaine. *Fundamentals of Molecular Spectroscopy*. New Delhi:Tata McGraw Hill, 2013.

Silverstein, M. Robert , Francis X. Webster and David Kiemle. *Spectrometric Identification of Organic Compounds*, New Delhi: Wiley, 2005.

Kemp, William. *Organic Spectroscopy*. New Delhi: Macmillan,1991.

BOOKS FOR REFERENCE

Barrow, M.Gordon. *Introduction to Molecular Spectroscopy*. New York: McGraw Hill, 1976.

Dudley, H. Williams and Ian Fleming. *Spectroscopic Methods in Organic Chemistry*. New Delhi: Tata McGraw-Hill, 2005.

Harris, C. Daniel. *Symmetry and Spectroscopy:An Introduction to Vibrational and Electronic Spectroscopy*. New York: Oxford University, 1980.

Pavia, L. Donald. *Introduction to Spectroscopy- A Guide for students of Organic Chemistry*. Singapore : Harcourt Asia, 2001.

Sathyanarayana, D.N. *Vibrational spectroscopy.* New Delhi: New Age, 2007.

Scheimann. *An Introduction to Spectroscopic Methods for Identification of Organic Compounds.* London: Pergamon Press, 1970.

JOURNALS

Journal of Spectroscopy
Journal of Molecular Spectroscopy
Journal of Applied Spectroscopy

WEB RESOURCES

http://www.astbury.leeds.ac.uk/facil/MStut/mstutorial.htm
http://www-keeler.ch.cam.ac.uk/lectures/Irvine/
http://www.nmr-relax.com/

PATTERN OF EVALUATION

CONTINUOUS ASSESSMENT:

Total Marks: 50 **Duration: 90 mins.**

Section A – 11 x 1 = 11 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match and answer in a line or two)

Section B – 3 x 8 = 24 Marks (3 out of 4 to be answered)
Section C – 1 x 15 = 15 Marks (1 out of 2 to be answered)

Third Component Tests:

List of evaluation modes:
Quiz
Seminars
Assignments
Problem Solving

END SEMESTER EXAMINATION:

Total Marks: 100 **Duration: 3 hours**

Section A – 20 x 1 = 20 Marks(All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match and answer in a line or two)
Section B – 5 x 8 = 40 Marks (5 out of 7 to be answered)
Section C – 2 x 20 = 40 Marks(2 out of 3 to be answered)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086

M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

ORGANIC SYNTHESIS AND PURIFICATION - PRACTICAL

CODE: 15CH/PC/P434 **CREDITS : 4**

L T P : 0 0 6

TOTAL HOURS : 78

Unit 1

Purification of Organic compounds- Paper Chromatography/TLC / Column chromatography (to be tested internally)

Unit 2

Organic Preparation

2.1 Single Step Preparations

- 2.1.1 Preparation of o-chloro benzoic acid (Sandmeyer reaction)
- 2.1.2 Preparation of methyl orange (Diazotisation)
- 2.1.3 Preparation of Benzpinacol (Photoreduction)
- 2.1.4 Preparation of Benzoicacid and benzyl alcohol (Cannizaro Reaction)
- 2.1.5 Preparation of Benzil (Oxidation)

2.2 Two Step Preparations

- 2.2.1 Preparation of p-bromo acetanilde from aniline (Acetylation, Bromination)
- 2.2.2 Preparation of s-tribromo benzene from aniline (Bromination, Reduction)
- 2.2.3 Preparation of m-nitroaniline from nitrobenzene (Nitration, Reduction)

2.3 Microwave assisted Preparations

- 2.3.1. Preparation of Fluorescein (Xanthene dye)
- 2.3.2. Preparation of Benzalacetophenone (Clasien Schmidt condensation)
- 2.3.3. Preparation of ethyl-2-cyano-3-(4-methoxy phenyl) propenoate (Knovenegal reaction)

Note : Spectroscopic identification / purification by chromatographic methods wherever applicable.

BOOKS FOR REFERENCE

Mohan, J. *Organic Analytical Chemistry – Theory and Practice.* New Delhi: Narosa, 2003.

Bansal, K. Raj. *Laboratory Manual of Organic Chemistry***.** New Delhi: Wiley Eastern, 2003.

Vogel, A.I. *Elementary Practical Organic Chemistry Part I, Small Scale Preparation.* New Delhi: CBS, 1998.

END SEMESTER EXAMINATION:

Total Marks: 50 marks **Duration : 6 hours**

Viva Voce : 10 marks

Procedure for the Preparation : 5 marks

Preparation : 35 marks

(i) Two Stage Preparation : (35 marks)

Quantity of Product 1 - 13 marks

Quantity of Product 2 - 13 marks

Quality of Final Product

a) Recrystallisation - 5 marks

b) Melting point - 4 marks

OR

(ii) Two Single Stage Preparations: (35 marks)

Quantity of Product - 7.5 marks (each)

Quality of Final Product

a) Recrystallisation - 5 marks (each)

b) Melting point - 5 marks (each)

TOTAL : 50 marks

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086

M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

SUMMER INTERNSHIP

CODE: 15CH/PN/SI32 **CREDITS: 2**

OBJECTIVES OF THE COURSE

- To enhance the experiential learning of the students by observing and hands on training at research institutes / chemical industries.
- To expose them to various experimental and analytical techniques employed in quality research.
- Enhance their skills in application - oriented courses.
- To familiarize the students to research ambience.

The Summer Internship programme is for a minimum period of one month. The students are expected to have regular attendance in their respective Institute and submit a report to the Department about their summer internship along with the attendance certificate. The students are expected to give a seminar presentation in the third semester of the work they have observed and conducted.

GUIDELINES FOR EVALUATION

The maximum marks for the Summer Internship is 50 and is divided into the following:

a) Summer Internship - Report	(20 Marks)
b) Seminar presentation	(20 Marks)
c) Attendance along with the log book	(10 Marks)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086

M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

ANALYTICAL INSTRUMENTATION

CODE: 15CH/PC/AI44 **CREDITS: 4**

L T P: 4 1 0

TOTAL TEACHING HOURS: 65

OBJECTIVES OF THE COURSE

- To equip the students with knowledge about different analytical techniques with a focus on their applications in industries and research laboratories
- To give an insight on the fundamental principles of analytical instrumentation techniques in order to pursue research

Unit 1

Spectroscopic Techniques **(15 hrs.)**

1.1 UV-Visible Spectroscopy- Principle and Instrumentation of Double Beam Spectrophotometer, Spectropolarimeters (Optical Rotatory Dispersion) and Spectrophotometer (Circular Dichroism)

1.2 Atomic Absorption and Emission Spectroscopy- Introduction, Principle and Instrumentation

1.3 Inductively Coupled Plasma Atomic Emission Spectroscopy (ICPAES) - Principle, Instrumentation and Applications

1.4 Infrared Spectroscopy- Dispersive and Fourier Transform- Principle and Instrumentation

1.5 Raman Spectroscopy- Principle and Instrumentation, Theory of Resonance Raman and Surface enhanced Raman Techniques

Unit 2 **(15 hrs.)**

Surface Characterization Techniques

Principle, Instrumentation and applications of -

2.1 Photoelectron Spectroscopy – Ultraviolet and X-Ray Photoelectron Spectroscopy (UPS and XPS), Auger Electron Spectroscopy (AES), ESCA

2.2 Electron Microscopy: Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM)

2.3 Probing Microscopy: Scanning Tunnelling Microscopy (STM), Atomic Force Microscopy (AFM)

2.4 Low Energy Electron Diffraction

Unit 3 **(15 hrs.)**

Electrochemical Techniques

Principle, Instrumentation and applications of -

3.1 Polarography (DC, AC and Pulse), Anodic and Cathodic Stripping Voltammetry.

3.2 Coulometry: Current- Voltage Relationship during Electrolysis, Coulometric Methods of Analysis, Potentiostatic Coulometry, Coulometric Titrations(Amperostatic Coulometry)

3.3 Amperometry, Amperometric Titrations, Biamperometry

3.4 Chronomethods: Chronoamperometry, Chronopotentiometry & Chronocoulometry

3.5 Cyclic Voltammetry

Unit 4

Thermoanalytical and Radiochemical Techniques **(14 hrs.)**

4.1 Thermogravimetry (TG), Differential Thermal Analysis. Differential Scanning Calorimetry

- Principle, Instrumentation, Factors affecting the Thermogram and Applications, Evolved Gas Analysis

4.2 Thermometric Titrations – Principle, Working and Applications

4.3 Radiochemical Methods: Hot Atom Chemistry – the Szilard - Chalmers Process, Neutron Activation Analysis - Principle, Instrumentation and Applications

Unit 5

Chromatography **(6 hrs.)**

5.1 Normal and Reversed Phase Liquid Chromatography (NP- and RP-LC), Gas Chromatography (GC) – Principle and Instrumentation, GC-MS – Applications

5.2 High Performance Liquid Chromatography (HPLC)- Principle, Instrumentation, Advantages and Applications

TEXT BOOKS

Sharma, B.K. *Instrumental Methods of Chemical Analysis*.Meerut: Goel, 2004.

Anjaneyulu, Y., Chandrasekhar.K and Valli Manickam. *A Text Book of Analytical Chemistry*. India: Pharma Book Syndicate, 2006.

Douglas, A. Skoog, James F.Holler and Niemen. *Principles of Instrumental Analysis*. Singapore: Haracourt Asia, 2001.

BOOKS FOR REFERENCE

Brown, R.D. *Introduction to Instrumental Analysis*. Singapore: McGraw Hill, 1987.

Eland**,** J.H.D. *Photoelectron Spectra*. London :Butterworths, 1984.

Douglas A.Skoog, Donald M West and James F Holler, Stanley R. Crouch. *Fundamentals of Analytical Chemistry*. New York :Saunders, 2004.

Ewing, W.Galen. *Instrumental Methods of Chemical Analysis*. New York: McGraw Hill,1985.

Bard, A.J and L.R.Faulkner. *Electrochemical Methods- Fundamentals and Applications.* New York:Wiley, 2006.

Fifield, F.W. and Kealy D. *Principles and Practice of Analytical Chemistry*. USA: Blackwell Science, 2004.

Gary D.Christian and James E. O'Reilly. *Analytical Chemistry.* New York :John Wiley, 2004.

JOURNALS

Journal of Analytical Chemistry
Journal of Spectroscopy
Journal of Electrochemistry

WEB RESOURCES
www.annualreviews.org/doi/abs/10.1146/annurev.pc.06.100155.001041

PATTERN OF EVALUATION

CONTINUOUS ASSESSMENT:

Total Marks: 50 **Duration: 90 mins.**

Section A – 11 x 1 = 11 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 3 x 8 = 24 Marks(3 out of 4 to be answered)
Section C – 1 x 15 = 15 Marks(1 out of 2 to be answered)

Third Component Tests:

List of evaluation modes:
Quiz
Seminars
Assignments

END SEMESTER EXAMINATION:

Total Marks: 100 **Duration: 3 hours**

Section A – 20 x 1 = 20 Marks (All questions to be answered, questions to be of objective type: MCQ, fill in the blanks, T/F, Match the following and answer in a line or two)

Section B – 5 x 8 = 40 Marks(5 out of 7 to be answered)

Section C – 2 x 20 = 40 Marks (2 out of 3 to be answered)

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600086

M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

ANALYTICAL INSTRUMENTATION - PRACTICAL

CODE: 15CH/PC/P542 **CREDITS: 2**

L T P : 0 0 3

TOTAL HOURS : 39

Unit 1
Colorimetry

1. Estimation of Vitamin- A / Cholesterol
2. Determination of stability constants of complexes

Unit 2
Spectrophotometry

3. Estimation of DNA / RNA
4. Simultaneous determination of caffeine and aspirin

Unit 3
Fluorimetry

5. Estimation of Riboflavin/Thiamine/ Fluorescein

Unit 4
Flame Photometry

6. Estimation of Sodium /Potassium

Unit 5
Thin Layer Chromatography

7. R_f determination and separation of a mixture of amino acids

Unit 6
Infrared spectroscopy [Demonstration]

9. Interpretation of IR spectra

BOOKS FOR REFERENCE

National Institute of Nutrition, ICMR. *A Manual of Laboratory Techniques*. Hyderabad: National Institute of Nutrition, 1983.

Plummer, David.T. *An Introduction to Practical Biochemistry*.New Delhi :Tata McGraw Hill, 2000.

Sadasivam, S. and Manickam A. *Biochemical Methods.*New Delhi: New Age

International, 1996.

Venkateswaran, V.,Veerasamy, R. Kulandaivelu A. R. *Principles of Practical Chemistry*. New Delhi : Sultan Chand, 1997.

END SEMESTER EXAMINATION:

Total Marks : 50 **Duration : 3hours**

Procedure = 10 (marks)

Viva voce = 10 (marks)

Reported value = 30 (marks)

Continuous assessment Internal:

Class Work = 30 (marks) – inclusive of *viva*

CA Test = 20 (marks)

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M.Sc. DEGREE: BRANCH IV- CHEMISTRY

SYLLABUS

(Effective from the academic year 2015 – 2016)

DISSERTATION

CODE: 15CH/PC/DI49

CREDITS: 9

GUIDELINES FOR DISSERTATION

Project should be done individually. Each student will choose a topic of her interest and the student will be assigned to a supervisor.

The project will require practical work with the submission of a project report. It should include experimental lab work. The duration of the project work is between 3 and 6 months

The project report should be submitted in the prescribed format containing a minimum of 50 pages. References should not be counted with the main pages. The report should be enhanced with graphs, spectra, tables and or photographs.

Each candidate has to give three periodical reviews to the internal guide on the scheduled dates prescribed by the department.

Each candidate can prepare 4 hard copies of the thesis. 1 copy for the candidate and 3 copies must be submitted to the department. The project should be submitted on the scheduled date prescribed by the Department. The student should appear for Viva-voce before a panel comprising the External Examiner, the supervisor and the Head of the Department.

GUIDELINES FOR EVALUATION

The maximum marks for the dissertation is 200 and **this will be converted to 100 marks by Controller of Examination**

Internal Evaluation: 100

* Attendance, log book, experimental work and project report

External Evaluation: 100

* Project report and *viva voce*