Paper 1 CH 101 (INORGANIC CHEMISTRY)

M.Sc. Chemistry Semester I Paper CH 101 Inorganic Chemistry

Hour-wise Synopsis

IC-01: Symmetry of Molecules **Dr. B. Sireesha**

1. **Concept of symmetry in Chemistry**: Introduction to symmetry, symmetry in nature, plants, leaves, flowers, animals, viruses, food, language, architecture, geometrical figures, polygons, pyramids, prisms and antiprisms, Molecular geometry, Concept of symmetry in molecules.
2. **Symmetry operation**: Operation, geometrical manipulation, equivalent and indistinguishable configurations, original and identical configurations of molecules. Operations- rotation, reflection and inversion. **Symmetry elements**: geometrical entity- point, line or plane in a molecule, five types of symmetry elements: Cn, σ, Sn, i and E.
3. **Rotational axis of symmetry C_n**: Rotation operation, axis, direction of rotation, notation with arrows, order of rotational axis, equivalent or indistinguishable orientations, identical orientation, e.g. H_2O, NH_3, $[Ni(CN)_4]^{2-}$, etc., types of rotational axis- Principal rotational axis, simple or secondary or subsidiary axes, e.g. BF_3, C_6H_6, planar ethylene, allene, etc., Cn axis n = 1,2,3,-,- , Cα axis, $Cn^n = E$.
4. **Plane of symmetry σ**: Reflection operation, bisecting plane, mirror images, e.g. H_2O, NH_3, etc., σ, $\sigma^2 = E$. Types of planes- a) vertical plane σv, e.g. H_2O, NH_3, BF_3, etc.; b) horizontal plane σh e.g. BF_3, C_6H_6, planar ethylene, etc. c) dihedral plane σd e.g. allene, regular tetrahedron, C_6H_6, etc., molecular plane, molecules with only plane of symmetry, e.g. HOD, C_6H_5OH, $POBrCl_2$ etc., molecules with no plane of symmetry, FClSO, PBrClFI etc.
5. **Improper rotational axis of symmetry S_n**: improper axis, rotational axis and perpendicular plane, order of improper axis, e.g. BF_3, eclipsed and staggered ethane, tetrahedron, etc., set of operations generated by S_n: molecules in which C_n axis is coincident with S_n axis, with same n order, with n = even order and n = odd order.
6. **Inversion centre *i***: Centre of symmetry, reflection operation through the center of gravity of molecule, direction, equivalent distance, equivalent atom, e.g. homo-diatomic molecules like H_2, O_2 etc, CO_2, C_2H_4 regular square planar and octahedral geometries, staggered ethane, chair form of cyclohexane, P_2F_4, etc., $i^2 = E$. **Identity element E**: doing nothing, rotation by 360°. Symmetry operations which give original orientation, identity operations C_n^n, S_n^n when n = even, S_n^{2n} when n = odd, i^n and σ^n, n = even.
7. **More about symmetry elements**, Cartesian coordinates system and symmetry elements, coordinate axes, inversion centre at origin, proper and improper rotational axes of symmetry and Cartesian axes, principal rotational axis, z axis in the Cartesian system, x and y axes, correlation between the symmetry elements, presence of other symmetry elements, notation by lower order of C_n, S_n when n is of even and odd order.
8. **Molecular point groups**: Molecules as points, definition, symbols, notation of point groups, generators, order of the point group *n*, number of symmetry elements in a point group *h*,, classification of molecules into point groups, **Type I point group:** Non-axial groups, C_1- asymmetric compounds, no symmetry elements, C_S- only σ generator, C_i- molecules with only centre of symmetry, examples of non axial point groups.

9. **Classification of point groups**: **Type II**: Molecules with only one axis of rotation, axial point group- C_n- molecules with only rotational axis as symmetry element, S_n- molecules with improper axis with even order greater then two, C_{nv}- molecules with one proper axis and n number of vertical planes, $C_{\alpha v}$, C_{nh}- molecules with one proper axis, horizontal plane and inversion centre, examples of the axial point groups.
10. **Classification: Type III;** Dihedral point groups, molecules with one n fold axis and n number of two-fold axis, D_n- molecules with only one n fold axis and n number of two-fold axis as symmetry elements, D_{nh}- molecules C_n, nC_2's $\perp$ C_n, σh and nσv's, *i* when n is of even order, D_{nd}- molecules C_n, nC_2's $\perp$ Cn, σd's and *i* when n is of odd order, $D_{\alpha h}$. Examples of dihedral point groups
11. **Classification: Type IV**: Molecules with more than one rotational axis of higher order than two-fold, polyhedral molecules, platonic solids, tetrahedron, octahedron, cube, dodecahedron and icosahedrons, T_d- molecules with four C_3 rotational axis and no other higher order axis. Oh- molecules with three C_4 rotational axis, I and I_h- molecules with several five fold axes. Examples of the polyhedral point groups.
12. **Classification**: Spherical point group, K_h. Systematic procedure for symmetrical classification of molecules into point groups, flow chart with examples. Exercises with the models of various molecules.
13. **Descent in symmetry with substitution**, substitutions on AB_3- planar, AB_4- tetrahedral, square planar and square pyramidal, AB_5- square pyramidal and trigonal bipyramidal, AB6- octahedral geometries, benzene, borazole etc.
14. **Exercises on molecular point groups** following the systematic procedure, working out point groups for common organic, inorganic and complex compounds.
15. **Symmetry and dipole moments**- molecules belonging to point groups C_n, C_S, C_{nv} possess permanent magnetic moment, **Symmetry criteria for optical activity**- dissymmetric and asymmetric molecules, molecules belonging to C_1, C_2, C_3, D_2 and D_3, diastereomers and mesomers.

M.Sc. Chemistry Semester I Paper CH 101 Inorganic Chemistry

Hour-wise Synopsis

IC 02: Bonding in Metal Complexes - I **Dr. P.Muralidhar Reddy**

Topics to be covered	No. of Hours
Crystal Field Theory-Salient features of CFT- Limitations and applications of crystal field theory (CFT)	1
d-orbital splitting patterns in regularOctahedral, and tetragonally distorted octahedral geometries, Jahn-Tellar theorem and its consequences	1
Crystal field splitting patterns intrigonal bipyramidal and square planar geometries	1
d-orbital splitting patterns in trigonal planar, Pentagonal bipyramidal, and linear geometries	1
Concept of weak field and strong fields-high spin and low spin octahedral complexes	1
Calculation of crystal field stabilization energies (CFSE's) in six and four coordinate complexes	1
Factors influencing the magnitude of crystal field in octahedral complexes	1
Origin of magnetism-Electron orbital motion-Electron spin motion- Definition of terms-magnetic dipole-polestrength- Gauss's Law and total magnetic induction	1
Magnetic Permeability- Magnetic susceptibility- Gram susceptibility-Molar susceptibility-Types of magnetic behavior	1
Classification of Magnetic behavior-Diamagnetism-Paramagnetism-Ferromagnetism-Antiferromagnetism-Ferrimagnetism-Curi temperature-Neel temperature	1
Calculation of magnetic momentfrom magnetic susceptibility spin only formula	1
Quenching of orbital angular momentum- Quenching of orbital angular momentum in octahedral complexes (spin free and spin paired complexes) - Quenching of orbital angular momentum in tetrahedral complexes	2
Determination of magnetic moment from Guoy's method	1
Applications of magnetic momentdata for the determination of oxidation states, bond type and stereochemistry. Spin crossover:High spin, low spin cross over phenomenon in $[Fe(Ophen)_2(NCS)_2]$ and $[Fe(R_2NCS_2)_3]$ Spinels.	1
	15hrs

M.Sc. Chemistry Semester I Paper CH 101 Inorganic Chemistry

Hour-wise Synopsis

IC 03: Coordination equilibria Dr. S.Sreekanth

Topics to be covered	**No. of Hours**
Solvation of metal ions- Metal complex formation in solution-Binary metal complexes – Demonstration using $CoCl_2$ and $CuSO_4$	1
Stability constants (types and relationships between them) – Step wise and over all stability constant. Kinetic stability and thermodynamic stability	1
Factors influencing the stability constants- Metal ion effects – effect of charge on metal ion, size of metal ion, charge/size ration, ionic potential, crystal field effect, and John-Teller effect	2
Pearson theory of hard and soft acids and bases (HSAB)- class A and Class B metals – effect of factors like electronegativity and softness on stability constant and symbiosis	2
Factors influencing the stability constants- Ligand effects – Basic nature of ligand, effect of substituent on ligand, steric effect,	1
Chelate effect – definition of chelation – effect of size of chelate ring and number of chelate ring formed.	1
Macrocyclic effect and cryptate effect – examples like crown ethers, cryptands, Macrocycles with pendent groups	1
Formation of macrocycles – size selectivity and concept of hole size match and its limitation	1
Methods used for the determination of Stability constants (Basic Principles only): pH metric method	1
Spectrophotometric method – mole ratio and jobs method	1
Polarographic methods – Polarography, diffusion current and stability constant relation	1
Ternary Metal Complexes – definition – Formation of ternary metal complexes – Step-wise and simultaneous equilibria with simple examples	2
	15hrs

M.Sc. Chemistry   Semester I   Paper CH 101   Inorganic Chemistry

Hour-wise Synopsis

IC – 04: Ligational Aspects of Diatomic molecules   Dr.M.Radhika

Topics to be covered	No. of Hours
Metal Carbonyls: Introduction, structure of CO, electronic configuration, CO as a ligand.	1
Molecular orbitals of CO: molecular orbital diagram of CO, electronic configuration of CO (sigma and pi molecular orbitals), discussion of energy of atomic orbitals of Carbon & Oxygen based on electronegativity, Bond order calculations. Donor and Acceptor molecular orbitals of CO : nature of bonding , anti- bonding &non bonding molecular orbitals, Donor and Acceptor molecular orbitals of CO .	1
Different types of bonding modes of CO : terminal mode with examples and bridging mode with examples. No. of electrons donated by CO in both modes, Reasons for the formation of bridging carbonyl complexes by only early transition metals.	1
Evidencefor multiple bonding , Infra- red spectroscopy- stretching frequencies for free CO, terminal CO and Bridging CO, reasons for decreasing order of stretching frequencies from free CO to terminal CO to Bridging CO. X-ray diffraction studies : measures the bond length and their trend in different types of bonding modes of CO.	1
18 Valence electron rule and its application : Definition, explanation of the rule with many examples (mononuclear and dinuclear metal carbonyl complexes). Its application in predicting the stability of the complexes.	2
Metal Nitrosyls: Introduction, structure of NO, electronic configuration, NO as a ligand.	1
Molecular orbitals of NO: molecular orbital diagram of NO, electronic configuration of NO (sigma and pi molecular orbitals), discussion of energy of atomic orbitals of Nitrogen& Oxygenbased on electronegativity, Bond order calculations. Donor and Acceptor molecular orbitals of NO : nature of bonding , anti- bonding &non bonding molecular orbitals, Donor and Acceptor molecular orbitals of NO .	1
Bonding modes of NO – terminal mode – linear & bent, bond angle , hybridization, no. of electrons donated; bridging mode , with examples.	1
Structuralaspects of [IrCl(PPh3)2(CO)(NO)]+ : binding mode of NO as a ligand, bond length, bond angle , hybridization, no. of electrons donated. [RuCl(PPh3)2(NO)2]: binding mode of NO as a ligand (different binding modes in one complex) , bond length, bond angle , hybridization, no. of electrons donated by 2 NO's . Stereo chemical control of valence in [Co(diars)2(NO)]2+ and Co(diars)2(NO)(SCN)]+.	1
Metal Dinitrogen complexes: - Introduction, structure of N_2, electronic configurationN_2 as a ligand	1
Molecular orbitals of N_2 : molecular orbital diagram of N_2, electronic configuration of N_2 (sigma and pi molecular orbitals), Bond order calculations. Donor and Acceptor molecular orbitals of N_2 : nature of bonding , anti- bonding &non bonding molecular orbitals, Donor and Acceptor molecular orbitals ofN_2	1
Bonding modes –Terminal and Bridging : side on , end on mode of binding, bond angle , hybridization, no. of electrons donated, with examples.	1
Stretching frequencies; Structures of Ru (II) and Os(II) dinitrogencomplexes; 18 electron rule	1
Chemical fixation of dinitrogen.: examples including synthesis of complexes	1

M.Sc previous teaching plans

STEREO CHEMISTRY (I –semester) Dr.B.Sakram

1st hr.: SYMMETRY- symmetry elements in methane, staggered ethane , ethylene

2nd hr.: Symmetry elements in benzene, chaircyclohexane ,allene , tartaric acid

3rd hr.: Point groups : Achiral and chiral point groups and their symmetry elements Desymmetrisation

4th. Axial, planar, helical chirality : Configurational nomenclature : Axially chiral allenes , spiranes.

5th hr.: Axial, planar, helical chirality· alkylidene , cycloalkanes , chiral biarylsatropoisomerism,

6th hr.: Planar chiral ansacompunds and trans – cyclooctene .

7thhr. helically chiral compounds

8th hr.: Relative and absolute configuration: Determination of absolute configuration

9th hr.: Anamolous X – ray scattering method and chemical correlation methods

10th hr.:Chemical correlation methods.

11th hr.: Properties of enantiomers and diastereoisomers : Discrimination of enantiomers based on diastereomeric interactions, chirotopical methods.

12th hr.: Chiral NMR solvents , chiral stationary phases and enzymatic methods

13th hr.: Racemisation ,racemate and resolution techniques: Resolution by direct crystallization , diastereoisomer salt formation , chiral chromatography and asymmetric transformation.

14th hr.: Determination of configuration in E,Z- isomers : Spectral , chemical methods.

15th h.: Determination of configuration in aldoximes and ketoximes.

NIZAM COLLEGE:DEPARTMENT OF CHEMISTRY

M.Sc. Chemistry Semester I Paper-II CH 101 T (Organic Chemistry)

Hour-wise Synopsis

OC-02: Reaction mechanism-I **Dr. A. Krishnam Raju**

1. **Electrophilic additions to carbon-carbon double bond: Introduction;** Stereoselective addition to carbon-carbon double bond;
2. *anti* addition-Bromination and epoxidation followed by ring opening.
3. *Syn* addition of OsO_4 and $KMnO_4$.
4. **Elimination reactions:** Type of elimination reactions; α-eliminations; β-eliminations; γ-eliminations; δ-eliminations; Pyrolytic eliminations; and photochemical eliminations.
5. **β-eliminations:** Types of β-eliminations: E2, E1, and E1CB mechanisms.
6. **E2 Mechanism:** Evidences for E2 Mechanism; Planarity of the Transition State in E2 reactions; Types of E2 Mechanisms; ANTI and SYN eliminations
7. Orientation and stereoselectivity in E2 eliminations; E2 reactions in cyclic compounds
8. Pyrolytic *syn* eliminations: Introduction and study of Pyrolytic syn eliminations with examples.
9. α-elimination: Introduction and study of α-eliminations with examples.
10. Elimination Vs substitution.
11. **Determination of reaction mechanism: I**ntroduction to Determination of reaction mechanism. Importance of determining reaction mechanism.
12. Energy profiles of addition reactions and Energy profiles of elimination reactions
13. Transition states
14. Isolation of Products and isolation of by-products: Chlorination on toluene in the presence of hν and under $AlCl_3$; Hofmann reaction; Sommelet reaction.
15. Structure of intermediates, use of isotopes, chemical trapping and crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

NIZAM COLLEGE : DEPARTMENT OF CHEMISTRY

LESSON PLAN FOR THE ACADEMIC YEAR 2017-2018 (Semester 1)

Class : M. Sc PREVIOUS **Section:** Organic Chemistry

Course/Paper: II Organic Chemistry,

Unit:conformational analysis(acyclic system) **No. of Hours Allotted**: 15

Topics to be covered	**No. of Hours required**
1. Introduction to the concept of dynamic stereochemistry. Conformational diastereoisomers and conformational enantiomers	1
2. Study of conformations in ethane and 1,2-disubstituted ethane derivatives like butane	1
3. dihalobutanes, halohydrin, ethylene glycol,	1
4. butane-2, 3-diol amino alcohols and 1,1,2,2-tetrahalobutanes.	1
5. Klyne-Prelog terminology for conformers and torsion angles	1
6. slip test	1
7. **Conformations of unsaturated acyclic compounds**: Propylene, 1-Butene, Acetaldehyde Propionaldehyde and Butanone.	1
8. **Factors affecting the conformational stability and conformational equilibrium**: Attractive and repulsive interactions.	1
9. Use of Physical methodsin conformational analysis.	1
10. Spectral methods in conformational analysis.	1
11. Steric and stereoelectronic factors-examples.Conformation and reactivity.	1
12 The Winstein-Holness equation	1
13. the Curtin – Hammett principle	1
Over view of the topic	**1**
Seminar by students	1
	15hrs

NIZAM COLLEGE : DEPARTMENT OF CHEMISTRY

LESSON PLAN FOR THE ACADEMIC YEAR 2017-2018 (Semester I)

Class : M. Sc previous **Section:** Organic Chemistry

Course/Paper: II- Organic Chemistry,

Unit: Natural products **No. of Hours Allotted**: 15

Topics to be covered	**No. of Hours required**
1. Introduction to Natural products	1
2.Importence of natural products as drugs	1
3.Isolation of natural products by steam distillation, solvent extract	1
4. Isolation of natural products by chemical products	1
5. General methods in structure determination of terpens. isoprene rules	1
6. Structure determinat and synthesis of terpenoil.	1
7.structure determination and synthesis of camphor	1
8.structure determination and synthesis of carotene	1
9.General methods of structure determination of alkaloids	1
10.General methods of structure determination of papaverine properties	1
11.quinine properties	1
12 Biogenesis of monoterpenes	1
13.Slip test	1
Over view of the topic	**1**
Seminar by students	1
	15hrs

Name of the Teacher: Mrs. G.Dhanalakshmi Head, Department of chemistry

Signature:

Name of the Topic	No. of hours required	Significance of the topic
Thermodynamics (15 H)		
Introduction to Thermodynamics	One hour	Important of thermodynamics in naturally occurring phenomena
Concept of Entropy, Entropy as a function of V and T, Entropy as a function of P and T.	One hour	The relationship between entropy and various parameters
Entropy change in isolated systems-Clausius inequality. Entropy change as criterion for spontaneity and equilibrium.	One hour	How entropy related to reversible and irreversible systems
Third law of thermodynamics. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases.	One hour	Pure crystalline substances also still exhibited randomness due to small impurities by using III law of thermodynamics for various phases
Standard entropies and entropy changes of chemical reactions. Thermodynamic relations. Gibbs equations.	One hour	Free energy relationship between entropy and chemical reactions
Maxwell relations. Gibbs equations for non-equilibrium systems	One hour	Various form of entropy , enthalpy and free energy relationship explained through Maxwell relations
Material equilibrium. Phase equilibium. Clausius-Clapeyron equation	One hour	Various phases are exhibited equilibrium process then a relationship between temperature with various parameters
Conditions for equilibrium in a closed system. Chemical potential of ideal gases. Ideal-gas reaction equlibrium-derivation of equilibrium constant.	One hour	For ideal gases evaluate the chemical potential relationship and equilibrium constant
Temperature dependence of equilibrium constant-the Van't Hoff equation	One hour	To deduced relationship between temperature and equilibrium constant through Vant Hoff's equation
Solutions: Specifying the Solution composition. Partial molar properties-significance.	One hour	Deduce the partial molar properties of solution with particular composition and their importance
Relation between solution volume and partial molar volume, measurement of partial molar volumes- slope and intercept methods	One hour	Relationship between partial molar volume through graphical method
The chemical potential. Variation of chemical potential with T and P	One hour	Explain the relation between chemical potential with temperature and pressure at constant volume
Gibbs-Duhem equation-derivation and significance	One hour	By using chemical potential of the system to deduce the Gibbs-Duhem equation-derivation and significance
Various numerical problems	One hour	All the concepts

Electrochemistry- I		
Derivation of Nernst equation – problems	Two hours	Deduce the Nernst equation and solve problems
Chemical and concentration cells (with and without transference)	One hour	Deduce the equations for both Chemical and concentration cells
Liquid junction potential (LJP) – derivation of the expression for LJP – its determination and elimination.	One hour	Explain the importance of Liquid junction potential (LJP) and deduce the expression for LJP.
Types of electrodes. Applications of EMF measurements	One hour	Explain the significance of electrodes and their applications in measured the EMF of the various types of solutions.
Solubility product, potentiometric titrations, determination of pH using glass electrode, equilibrium constant measurements	One hour	Deduce equation for the solubility product, potentiometric titrations (acids Vs strong base etc.) pH, and equilibrium constant.
Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration over-potential	Two hours	Explain the decomposition potential and its significance. Electrode polarization – its reasons and removal. Concentration over-potential
Concept of activity and activity coefficients in electrolytic solutions, and the mean ionic activity coefficient	One hour	Explain the theory of activity and activity mean ionic activity coefficients and deduced the equations of electrolytic solutions
Debye-Huckel theory of electrolytic solutions. Debye-Huckel limiting law (derivation not required)	One hour	Explain the theory of Debye-Huckel theory of electrolytic solutions and deduce the equation.
Calculation of mean ionic activity coefficient. Limitations of Debye-Huckel theory. Extended Debye-Huckel law	One hour	Problems solve the mean ionic activity coefficient. Explain the limitations of Debye-Huckel theory and extended Debye-Huckel law.
Theory of electrolytic conductance.	One hour	Explain the theory of electrolytic conductance of solutions with examples.
Derivation of Debye-Huckel-Onsager equation – its validity and limitations	One hour	Give details of the theory and derive the equation for Debye-Huckel-Onsager equation. Explain the strength and boundaries of the Debye-Huckel-Onsager equation
Concept of ion association – Bjerrum theory of ion association (elementary treatment)-ion association constant – Debye-Huckel-Bjerrum equation	Two hours	Explain the concept and theory of the ion association with primary treatment. Deduce the ion association constant via Debye-Huckel-Bjerrum equation.

Quantum Chemistry – 1		
A brief review of Black body radiation	One hour	Black body radiation is origin of quantum mechanics
Planck's concept of quantization-Planck's equation average energy of an oscillator	One hour	Various theories are explain to find out energy of and oscillator at lower and higher energy levels split under electromagnetic radiation of an atom or a molecule
Wave particle duality and uncertain principle-significance of these for microscopic entities and problems	One hour	The relation between frequency and mass of the microscopic particle. At a time not find out the position and momentum of a particle and problem related to both the concepts.
Emergence of quantum mechanics. Wave mechanics and Schrödinger wave equation	One hour	Classical mechanics has been failed explained the properties of microscopic particles then the origin of quantum mechanics. Separation of variable and evaluate the amplitude equation and from this deduced the Schrodinger wave equation.
Operators- Operator algebra. Commutation of operators, linear operators. Complex functions.	One hour	Introduction of operators and inter-linking of an operator with wave function. How to use mathematical operators to quantum chemistry applications
Hermitian operators. Operators ∇ and ∇^2.Eigen functions and eigenvalues. Degeneracy. Problems	One hour	Hermitian operators are how to correlate with real and orthogonality nature. Operators ∇ and ∇^2 importance. Any function become eigen function which conditions are follow the operator and problems
Linear combination of eigen functions of an operator. Well behaved functions. Normalized and orthogonal functions	One hour	The correlation between N numbers of eigen functions with an operator to obtained an eigen value function. If any wave functions are called well-behaved functions certain conditions are followed then that functions used in quantum mechanics. Explain the conditions for Normalization and orthogonal conditions.
Postulates of quantum mechanics	One hour	Physical interpretation of wave function. Observables and Operators. Measurability of operators. Average values of observables.
The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation	Two hour	For the time dependent Schrodinger equation considered time independent equation and the time-independent Schrodinger equation considered time dependent equation

		and how to separation of variables.
Theorems of quantum mechanics. Real nature of the eigen values of a Hermitian operator significance	One hour	Importance of theorems of quantum mechanics. Significance of Hermitian operator and eigen value function
Orthogonal nature of the eigen values of a Hermitian operator-significance of orthogonality. Expansion of a function in terms of eigenvalues. Eigen functions of commuting operators- significance. Simultaneous measurement of properties and the uncertainty principle and problems	One hour	Two different wave function with a Hermitian operator then verify the orthogonality and commuting operator is used to eigen functions and deduce the eigen values of respective eigen functions. Applied the uncertainty principle to eigen functions and solve the problems related to eigen function value.
Particle in a box- one dimensional and three dimensional.	One hour	By using well-behaved conditions to deduce the energy and wave function equation by using boundary conditions of the particle in a one dimensional box and three dimensional box.
Plots of $\bigtriangledown$ and $\bigtriangledown^2$-discussion. Degeneracy of energy levels. Calculations using wave functions of the particle in a box orthogonality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules.	Two hours	Graphical representation for energy levels of particle in one and three dimensional box. Using wave functions of particle one and three dimensional box to deduce normalization constants and verify the orthogonality and calculate the energy, position and momentum and probabilities of electron density. Linear polyene molecules are applicable for particle in one dimensional box.

Chemical Kinetics- I		
Theories of reaction rates: Collision theory and steric factor, Transition state theory	One hour	Explain the theories of reaction rates of both Collision and Transition state and deduce the equations.
Thermodynamic formulation of transition state theory. Potential energy surface diagram, Reaction coordinate, Activated complex. Activation parameters and their significance.	One hour	Deduce equation for the thermodynamic formulation of transition state theory and explain the Potential energy surface diagram, Reaction coordinate, Activated complex. Activation parameters and their importance
The Eyring equation. Unimolecular reactions and Lindamann's theory.	One hour	Deduce the Eyring equation and explain the Unimolecular reaction with various conditions and Lindamann's theory.
Complex reactions- Opposing reactions, parallel reactions and consecutive reactions (all first order type)	One hour	Explain the complex, opposing, parallel and consecutive reactions of first order rate constant with examples.
Chain reactions, general characteristics, steady state treatment. Example- H_2-Br_2 reaction. Derivation of rate law	Two hours	Discuss the chain reaction their features and apply the steady state treatment and apply the H_2-Br_2 reaction and it's deduce the equation.
Effect of structure on reactivity- Linear free energy relationships	One hour	Explain the linear free energy relationships with effect of structure on reactivity.
Hammett and Taft equations- substituent (σ and σ^*) and reaction constant (ρ and ρ^*) with examples	One hour	Deduce the Hammett and Taft equations with various substituent and reaction constant with different examples.
Deviations from Hammett correlations, reasons - Change of mechanism, resonance interaction	One hour	Reasons of Abnormalities of Hammett correlations and modifications of mechanism and resonance interaction.
Taft four parameter equation. Correlations for nucleophillic reactions	One hour	Explain the Taft four parameter equation and their correlation with nucleophilic reactions.
The Swain – Scott equation and the Edward equation	One hour	Deduce the equations for Swain – Scott and Edward equation
Reactions in solutions: Primary and secondary salt effects	One hour	Explain the primary and secondary salt effects
The reactivity-selectivity principle – Isokinetic temperature - Isoselectivty rule, Intrinsic barrier.	Two hour	Explain the principle of isokinetic temperature reactivity-selectivity, isoselectivity rule and intrinsic barrier.
Hammond's postulate	One hour	Explain the Hammond's postulate.

LESSON PLAN FOR THE ACADEMIC YEAR 2017-2018 (Semester I)

Class : M. Sc Previous **Section:** Chemistry

Course/Paper: IV- **Paper CH 104** (ANALYTICAL TECHNIQUES and SPECTROSCOPY - I)

Unit: ASP 01: Techniques of Chromatography **No. of Hours Allotted**: 15

Topics to be covered	No. of Hours
Separation Methods: Introduction to separation methods, types of separation methods, introduction to chromatographic methods– classification, stationary and mobile phases;	1
Principle of chromatography – adsorption, partition, differential migration rates, partition ratio, partition coefficient, capacity factor, selectivity factor; problems	1
Theoretical considerations: Retention time, Retention volume, adjusted retention time, adjusted retention volume, relation between partition ratio and retention time. Problems.	1
Efficiency of separation: Resolution of chromatographic peaks, diffusion. Problems on resolution. Factors effecting the separation.	1
Rate theory and Plate theory: **Rate theory** – Van de Meter's equation – multiple path effect- Eddy diffusion, Longitudinal diffusion and mass transfer.	1
Plate Theory: concept of theoretical plates in the column – equilibrium steps, resolution based on the number of theoretical plates, calculation of N efficiency, Height equivalent to theoretical plates (HETP - H), relation between N and H. Problems.	1
Gas Chromatography (GC) – Principle of GC, instrumentation, carrier gas as mobile phase – characteristics; sample injection; types of columns – Packed and Capillary / Open tubular columns – Classification of Capillary columns – WCOT, SCOT, PLOT;.	1
Stationary phases in GC – solid and liquid stationary phases; Detectors – use of detectors, signal-to-noise ratio, types of detectors – TCD, FID and ECD	1
Derivatization techniques: uses / advantages of derivatization, types of derivatization – acylation, silylation and alkylation – reagents used.	1
Programmed Temperature GC (PTGC): Methodology of PTGC, difference between GC and PTGC; **applications of GC –** methods of quantification – external and internal standard methods; Analysis of Hydrocarbons in mixture by GC	1
Applications: Assay of methyl testosterone in tablets, determination of atropine in eye drops.	1
High Performance Liquid Chromatography (HPLC): introduction, principle of HPLC, instrumentation – sample injection – loop and valve injection, requirement for high pressure, columns – guard column, stationary phases and mobile phases.	1
Classification of HPLC based on stationary phases – normal phase HPLC, reverse phase HPLC – polar, non-polar and intermediate polar stationary phases.	1
Mobile phases, types of elution – isocratic and gradient elution. Detectors – uses, types of various detectors in HPLC –UV detector, fluorescence detector and photodiode array detector..	1
Applications of HPLC - Assay of aspirin, paracetamol tablets. Discussion of chromatography techniques.	1
	15hrs

Name of the Teacher**: Dr. A.V.Aparna** Head, Department of Chemistry

Signature: Signature:

Unit: ASP 02: NMR Spectroscopy – I (^{1}H – NMR) **No. of Hours Allotted**: 15

Topics to be covered	**No. of Hours**
Introduction to Spectroscopy, electromagnetic spectrum,Magnetic properties of nuclei	1
Principles of NMR Instrumentation, CW and pulsed FT instrumentation	1
Equivalent and non equivalent protons, enantiotopic and diastereotopic protons	1
Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects,	2
Signal integration, Spin-spin coupling: vicinal, germinal and long range - examples	1
Coupling constants and factors affecting coupling constants	1
Applications of ^{1}H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions),	2
E, Z isomers, conformation of cyclohexane and decalins	1
keto-enol tautomerism, hydrogen bonding	1
proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation.	1
Magnetic resonance imaging (MRI)	1
1H NMR of organic molecules and metal complexes: ethyl acetate, 2- butanone, mesitylene, paracetamol, asprin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, [HNi(OPEt3)4]+, [HRh(CN)5] (Rh I=1/2), [Pt(acac)2].	2
	15hrs

Name of the Teacher**: Dr. T.Gangadhar** Head, Department of Chemistry

Signature: Signature:

Unit: ASP 03: Rotational, Microwave and Raman Spectroscopy No. of Hours Allotted: 15

Topics to be covered	No. of Hours
Introduction to spectroscopy, electromagnetic spectrum, Molecular Spectroscopy – types of molecular energies – Rotational, Vibrational, Electronic and Translational energies	1
Microwave Spectroscopy – Introduction, electronic, Vibrational and Rotational levels – transitions between rotational energy levels – microwave region, selection rules, instrumentation of microwave spectrometer.	1
Classification of molecules based on moment of Inertia – linear molecules, symmetric tops, spherical tops and asymmetric tops. Rigid Rotor Model - diatomic molecule as rigid rotor.	1
Rigid Rotor Model –,rotational energies of diatomic molecules, interaction of radiation with molecules, Determination of moment of inertia and bond length from rotational spectra.	1
Isotopic effect on rotational spectra, calculation of atomic mass from rotational spectra, problems.	1
Vibrational Spectroscopy – principle, Vibrational energy levels of diatomic molecules, Vibrational motion of systems that behave classically – stretched, compressed and rest levels, selection rules of IR, IR active and IR inactive molecules.	1
Restoring force, force constant, calculation of force constant, anharmonic nature of vibrations, interaction of radiation with vibrating molecules, fundamental bands, overtones, hotbands, combination and difference bands	1
Fluctuation of dipole moment due to asymmetric and bending modes of vibration, modes of CO_2 molecule.	1
Vibrations of polyatomic molecules – symmetric stretching, symmetric bending and antisymmetric stretching – vibrations of H_2O molecule.	1
Concept of group frequencies – characteristics of Vibrational frequencies of functional groups.	1
Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding.	1
Isotopic effect on group frequencies, IR spectra of metal coordinated NO_3^-, SO_4^{-2}, CO_3^{-2} ions.	1
Raman Spectroscopy – Introduction, principle, selection rules, Raman Effect – Classical theory of Raman Effect **.**	1
Quantum theory of Raman Effect, Rotational and Vibrational Raman Spectra, Stokes and Anti-Stokes lines.	**1**
Complementary nature of IR and Raman Spectroscopic techniques. Discussion	**1**
	15hrs

Name of the Teacher**: Dr. A.V.Aparna** Head, Department of Chemistry

Signature: Signature:

Unit: ASP 04: Electronic spectroscopy **No. of Hours Allotted**: 15

Topics to be covered	**No. of Hours**
Introduction to Spectroscopy, EMR, types of spectroscopy	1
Electronic spectra: Elementary energy levels of molecules	1
Selection rules for electronic spectra; types of electronic transitions in molecules	1
Beers law, lamberts law, deviations	1
Chromophores - definition, examples, Congugated dienes, trienes and polyenes	2
Unsaturated carbonyl compounds, benzene and its derivatives, Woodward-Fieser rules.	2
Woodward-Fieser rules, examples	1
Polynuclear aromatic hydrocarbons and diketones. Solvent and structural influences on absorption maxima	1
Stereochemical factors. Cis-trans isomers, and cross conjugation	1
Application of electronic spectra of metal complexes: $3d^1$ and $3d^9$ hexaaquo metal complexes.	1
Quantitative applications of electronic spectroscopy: Beer’s law application to mixture analysis	2
dissociation constant of a weak acid, Charge transfer spectra	1
	15hrs

Name of the Teacher**: Dr. P.Someshwar** Head, Department of Chemistry

Signature: Signature:

Sem-2

Paper CH 201 INORGANIC CHEMISTRY

M.Sc. Chemistry Semester II Paper CH 201 Inorganic Chemistry

Hour-wise Synopsis

IC – 05: Reaction mechanisms of transition metal complexes Dr.P.Muralidhar Reddy

Topics to be covered	No. of Hours
Ligand substitution reactions-Energy profile of a reaction- Endothermic reactions-Exothermic reactions-Transition state or Activated Complex – Reaction energy-Electrophilic agent-Nucleophilic agent	1
Classification of reaction mechanism-Types of substitution reactions (SE, SN, SN^1, SN^2). Langford and Grey classification – A mechanism, D-Mechanism, Ia, Id, and Intimate mechanism.	1
Substitution reactions in octahedral complexes- Nucleophilic substitution reactions-Electrophilic substitution reactions-SN^1 mechanism-SN^{II} mechanism-Pictorial representation of SN^1 and SN^2 reaction	1
Ligand substitution reactions in octahedral complexes:Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis-charge on the substrate- effect of leaving group- effect of inert ligand- steric hindrance – chelate effect	1
Base Hydrolysis,Conjugate Base (SN^1CB) Mechanism, and Evidences in favor of SN^1CB Mechanism.Pictorial representation of SN^1CB reaction	1
Substitution reactions with out Breaking Metal-Ligand bond. Anation reaction	1
Ligand Substitution reactions in Square-Planar complexes: Mechanism of Substitution inSquare-Planar complexes- Trans-effect, Trans-influence, and Trans-effect series.	1
Theories of Trans-effect - Grienberg's Polarization theory and Π - bonding theory	1
Applications of Trans-effect in synthesis of Pt (II) complexes	1
Electron Transfer Reactions (or Oxidation-Reduction Reactions or Redox reactions) in Coordination compounds	1
Mechanism of One-electron Transfer Reactions – classification-Introduction of Inner SphereMechanism and Outer Sphere Mechanism	1
Atom (or group) Transfer or Ligand bridge mechanism or Inner SphereMechanism	1
Direct electron Transfer or Outer Sphere Mechanism. – Self exchange reaction and cross exchange reaction.	1
Factors affecting directelectron transfer reactions	1
Cross reactions and Marcus-Hush theory	1
	15hrs

M.Sc. Chemistry Semester II Paper CH 201 Inorganic Chemistry

Hour-wise Synopsis

IC 05: Bonding in metal complexes-II

Dr. B.Sireesha

1. **Free ion Terms and Energy levels**: Energy levels in an atom- n, l, m, m_S. Configuration of the free ion, energy state of the atom, terms, inter electronic repulsion perturbations and spin-orbit coupling perturbations, microstates.

2. **Microstates:** formulae for calculating number of microstates, general equation, equations for equivalent electrons, inequivalent electrons, calculation of microstates for p^n and d^n configurations.

3. Orbital angular momentum of the electron ***l***, and resultant orbital angular momentum Σl = L, notation of terms χ, vector coupling of orbital angular momenta, p-p configuration- p^2, p^3, p-d configuration-p^1d^1, d-d configuration- d^2.

4. Spin angular momentum of the electron $\mathbf{m_S}$, and resultant spin angular momentum Σm_S= S, two electron configurations- p^2 and d^2 cases, three electron configurations- p^3 and d^3 cases. Spin orbit coupling- theory, types- phenomenon of L-S (Russell-Saunders) coupling scheme, j-j coupling scheme.

5. **Russell- Saunders or L-S coupling scheme**: Spin orbit coupling constant J, number of J values calculation, vector coupling of orbital and spin angular moments for p^2 configurations, representation of term symbols, spin multiplicities, p^1d^1 configuration, **j-j coupling scheme**: inter-electronic repulsion parameters of some transition metal complexes.

6. **Derivation of Terms** using the allowed values of m_l and m_S values for single electron p^1 and d^1 configurations, and p^2 configuration, calculation of M_L, M_S and single electron wave functions for all microstates, summary of microstates table, assignment of Terms.

7. **Derivation of Terms** for p^3 configuration, calculation of M_L, M_S and single electron wave functions for all microstates, summary of microstates table, assignment of Terms.

8. **Derivation of Terms** for d^2 configuration, calculation of M_L, M_S and single electron wave functions for all microstates, summary of microstates table, assignment of Terms.

9. Illustration of subtraction process of array of tables for p^n and d^n configurations,. Derivation of terms symbols for a closed sub-shells, s^2, p^6, d^{10} and f^{14} configurations, ^1S. **Hole formalism**: Hole formulation, spin factoring, holes equivalent to number of unpaired electrons in half filled and completely shells.

10. Terms for all s^n, p^n and d^n configurations. **Energy ordering of terms**- Hund's rules for the determination of ground state Terms, comparison of the J-terms in d^2 and d^8 configuration. The complete profile of energy level splitting for d^2 configuration showing 45 microstates.

11. **Inter electron repulsion parameters**: Racah parameters- A, B and C, Condon-Shortley parameters- F_0, F_2 and F_4. Relation between the two parameters, Energies of the terms of d^2 configuration, Racah parameter values for some metal ions.

12. **Spin-orbit coupling parameters**: zeta ζ and lambda λ, dependence of zeta on n and *l* quantum numbers, zeta values of some 3d and 4d metal ions, relationship between ζ and λ.

13. Symmetry of atomic orbitals and spectral Terms- symmetry species of atomic orbitals and irreducible representations, symmetry species of Terms, rules for the use of g and u in irreducible representations. Determination of Ground State Term symbol for a given electronic configuration.

14. Construction of ligand field energy level diagrams, **Effect of weak cubic (octahedral and tetrahedral) fields** on S and P terms. Effect of weak cubic (octahedral and tetrahedral) fields on D terms in d^1, d^4, d^6 and d^9 configurations. Shapes of f-orbitals, splitting of f-orbitals in octahedral and tetrahedral crystal fields.

15. Effect of weak cubic (octahedral and tetrahedral) fields on F terms in d^2, d^3, d^7 and d^8 configurations. **Orgel diagrams**: definition, classification of Orgel diagrams into three sets- a) d^1, d^4, d^6 and d^9 configurations, b) d^2, d^3, d^7 and d^8 configurations and c) d^5 configuration. Use of Orgel diagrams in the assignment of electronic transitions and calculating the energy of the transitions.

M.Sc. Chemistry Semester II Paper CH 201 Inorganic Chemistry

Hour-wise Synopsis

IC 07: Metal clusters M. Radhika

Topics to be covered	**No. of Hours**
Carbonyl clusters: Introduction, Bonding- synergic mechanism, structures of mono & di-carbonyls	1
Factors favoring Metal-Metal bonding – Classification of Clusters – Low nuclear & high nuclear metal clusters, with examples.	1
Low NuclearityClusters : M3 and M4 clusters , structural patterns in M3(CO)12 (M=Fe,Ru,Os) and M4(CO)12 (M=Co,Rh,Ir) Clusters, No. of M-M bonds, Co ligation as terminal and bridged form	1
Metal carbonyl scrambling : Concept of fluxionality, ^{1}H-NMR importance in fluxionality, stability of the complex during scrambling, examples.	1
High Nuclearity clusters M5, M6, M7, M8 and M10 Clusters: structural patterns, , No. of M-M bonds, Co ligation as terminal and bridged form	1
Polyhedral skeletal electron pair theory and Total Electron Count theory – Capping rule : Wades rules and TEC theory explanation with many examples including both low nuclear and high nuclear complexes. Definition for Capping rule and Classification with different examples.	2
Structural patterns in [Os6(CO)18]2- , [Rh6(CO)16], {Os7(CO)21] , {Rh7(CO)16]3-, [Os8(CO)22]2-, [Os10C(CO)24]2- and [Ni5(CO)12]2-, application of Wades rules to classify these complexes as closo, nido and arachano structures.	1
Metal Halide clusters: Introduction, and classification to types in Dinuclear Metal-Metal systems – Edge sharingBioctahedra, Face sharing Bioctahedra, Tetragonal prismatic and Trigonal antiprismatic structures	1
Edge sharing Bioctahedra, Face sharing Bioctahedra : Structural aspects with examples	1
Tetragonal prismatic and Trigonal antiprismatic structures : Structural aspects with examples	1
Structure and bonding in [Re2Cl8]2-: formation of sigma, pi and delta bonds, orbitals involved, structural features and bonding of carbonyls.	1
Octahedral halides of [Mo6(Cl)8]4+ and [Nb6(Cl)12]2+. : structural aspects	1
Hoffman’s Isolobal analogy and its Structural implications. : Isolobal analogy definition, symbol for analogy, different analogous fragments both in organic and inorganic chemistry, applications	1
Boranes, carboranes, : similarities, types of carboranes .STYX Rule. : definition, rules to be followed to write the short hand notation of structures of boranes.	1

M.Sc. Chemistry Semester II Paper CH 201 Inorganic Chemistry

Hour-wise Synopsis

IC 08: Biocoordination chemistry Dr. Ashwini.K

Topic to be covered	**No. of hours**
Introduction to Bio coordination chemistry, interface of biology and chemistry	**1**
Essential and non-essential metals. Role of metal ions in human health and well being, important role of each metal	**1**
Effect of metal ion concentration-deficiency symptoms and overdose effects	**1**
Principles behind the selection of these metals by nature	**1**
Oxygen transport carriers- introduction to structure of the porphyrin ring and metal centre in hemoglobin, Myoglobin .	**1**
Classification of proteins into primary, secondary and tertiary structures, mechanism of oxygen transport.	**1**
Models of oxygen binding-griffith model, weiss model, Electronic aspects of dioxygen binding	**1**
Cooperativity in oxygen transport, role of globin chain	**1**
Transport of NO and CO_2-harmful effect of CO binding	**1**
Bohr effect-oxygen binding curves, Hill constant, role of DPG	**1**
Comparision of Hb and Mb-in transport and storage of dioxygen	**1**
Photosynthesis- introduction, importance, relevance to mankind and chemistry in particular, structure of chloroplast-grana and stroma	**1**
Photolysis of water, electron transport,generation of ATP +NADPH, liberation of dioxygen, Z-scheme	**1**
Vitamin B6 models-structure and mechanism,transaminations	**1**
Mechanism of Decarboxylation and dealdolation	**1**
total	**15**

M.Sc. Chemistry Semester II CH 202 T (Organic Chemistry)

Hour-wise Synopsis

OC-05: Reaction mechanism-II **Dr. A. Krishnam Raju**

1. **Nucleophilic Aromatic substitution:** Introduction ; S_N1 (Ar) and S_N2 (Ar) reactions and their mechanisms
2. Benzyne mechanisms;
3. Evidence for the structure of benzyne.
4. Von Richter rearrangement.
5. Definition and types of ambident nucleophiles.
6. **Neighbouring group participation:** Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration
7. Isotopic labeling and cyclic intermediates
8. Neighbouring group participation involving Halogens
9. Neighbouring group participation involving Oxygen
10. Neighbouring group participation involving Sulphur and Nitrogen
11. Neighbouring group participation involving Aryl and Cycloalkyl groups
12. Neighbouring group participation involving σ and π- bonds.
13. Introduction to non-classical carbocations.
14. **Electrophilic substitution at saturated carbon and single electron transfer reactions.** Mechanism of aliphatic electrophilic sustitution. S_E1 and SE2 mechanisms.
15. S_E^i and SET mechanism.

PERICYCLIC REACTIONS (II SEMESTER) Dr.B.Sakram

1st hr.: Definition and characteristics of pericyclic reactions .

2nd hr.: classification of pericyclic reaction.

3rd hr.: Aromatic transition state approach (ATS) guidelines.

4th hr.: Applications of ATS approach to pericyclicreactions:application of ATS to electrocyclisation, electrocyclic ring opening reaction, selection rules.

5th hr.: Application of ATS approach to cycloaddition /cycloreversion reactions and selection rules.

6thhr.: Application of ATS approach to sigmatropic reactions and selection rules .

7th hr.: Frontier molecular orbital (FMO) approach guide lines.

8th hr.: Molecular orbital diagrams of various number of P-orbitals.

9th hr.:Application of FMO approach to Electrocyclisation/Electro cyclic ring opening reactions and selection rules.

10th hr.: Application of FMO approach to cyclo addition/Cyclorevertion reaction and selection rules.

11th hr.: Application of FMO approach to sigmatropic reaction and selection rules.

12th hr.: Conservation method/Corelation Diagram(C D) approach guide lines.

13th hr.: Applications of CD approach to Electrocyclisation/Electro cyclic ring opening reactions and selection rules.

14thhr.:Applications of CD approach tocyclo addition/Cyclorevertion reaction and selection rules.

15th hr.:Solving problems on Pericyclicreactions .

NIZAM COLLEGE: DEPARTMENT OF CHEMISTRY

LESSON PLAN FOR THE ACADEMIC YEAR 2017-2018 (Semester II)

Class : M. Sc Previous **Section:** Organic Chemistry

Course/Paper: II- CH(OC) 301T: Organic Chemistry,

Unit: photochemistry **No. of Hours Allotted**: 15

Topics to be covered	**No. of Hours required**
introduction	1
Photochemistry of π-π* transitions: Excited states of alkenes, cis-trans isomerisation,	1
photo stationary state. Photochemistry of 1,3-butadiene	1
Electrocyclisation rearrangement	1
sigmatropic rearrangements, di-π methane rearrangement.	1
Intermolecular reactions, photocycloadditions	1
Working of examples	1
photodimeriastion of simple and conjugated olefins.	1
Addition of olefins to α, β-unsaturated carbonyl compounds. Excited states of aromatic compounds,	1
Photoisimerisation of benzene. **Photochemistry of (n-π*) transitions Excited states of carbonyl compounds,**	1
homolytic cleavage of α- bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkane diones.	1
Intermolecular abstraction of hydrogen: photoreduction-influence of temperature, solvent, nature of hydrogen donor and structure of the substrate.	1
Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2 diketones,	1
Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.	**1**
Overview of the topic	1
	15hrs

Name of the Teacher: Mrs.P.Revathi Head, Department of chemistry

Signature:

NIZAM COLLEGE: DEPARTMENT OF CHEMISTRY

LESSON PLAN FOR THE ACADEMIC YEAR 2017-2018 (Semester II)

Class : M. Sc Previous **Section:** Organic Chemistry

Course/Paper: II- CH(OC) 301T: Organic Chemistry,

Unit: Reactive intermediates and molecular rearrangements **No. of Hours Allotted**: 15

Topics to be covered	**No. of Hours required**
1. Introduction	1
2.**CARBOCATION:** Generation, detection,structure and reactions of carbocation.	1
3.**CARBANION**:Generation,detection,structure and reactions of carbanion.	1
4.**CARBENE**: Generation,detection,structure and rectations of carbene.	1
5.**NITRENE:** Generation,detection,structure and rectations of nitrene.	1
6. **FREE RADICALS**: Generation,detection,structure and rectations of free radicals.	1
7.**MOLECULAR REARRANGEMENT**: Introduction,Defenation and classification	1
8. MOLECULAR REARRANGEMENTS INVOLVING ***i)Electron deficient carbon***: a)Wagner Meerwein rearrangement b)Pinacol-pinacolone rearrangement	1
9. c)Allylic rearrangement d)Wolf rearrangement **MOLECULAR REARRANGEMENTS INVOLVING** ***ii)Electron deficient Nitrogen:*** a)Hoffmann rearrangement	1
10. b)Lossen rearrangement c)Curtius rearrangement d)Schmidt rearrange	1
11. e)Beckmann rearrangement **MOLECULAR REARRANGEMENTS INVOLVING** ***iii)Electron deficient Oxygen*****:** Baeyer Villiger Oxidation reactions	1
12. Base Catalysed Rearranments: Benzilic acid rearrangemnt Favourskii rearrangement	1
13. Transannular rearrangement Sommelett-Hauser rearrangement , Smiles rearrangment	1
Over view of the topic	**1**
Seminar by students	1
	15hrs

Name of the Teacher: Mr.G.Dhanalakshmi Head, Department of chemistry

Signature:

Name of the Topic	No. of hours required	Significance of the topic
Thermodynamics-II & Statistical Thermodynamics		
Ideal solutions. Thermodynamic properties of ideal solutions	One hour	Thermodynamic properties of ideal solutions discussion and deduce the equations
Mixing quantities. Vapour pressure - Raoult's law	One hour	Explain the Raoult's law applied to ideal solutions and deduce the equations
Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law	One hour	Explain the thermodynamic properties of ideally dilute solutions and derive the equation for vapor pressure through Henry's law
Nonideal systems. Concept of fugacity, fugacity coefficients. Determination of fugacity	One hour	Discussion on non-ideal systems and introduction of fugacity and deduce the equations for fugacity.
Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non ideal solutions.	One hour	For non-ideal solution deduce the activity coefficient equation
Determination of activity coefficients from vapour pressure measurements.	One hour	Using activity coefficient equation calculate the vapor pressure
Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation.	One hour	Apply the activity coefficient equation to Gibbs-Duhem equation
Multicomponent phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation	Two hours	For a multi-component phase equilibrium state to evaluate the lowering vapor pressure and depression freezing point and elevation of boiling point
Partition Functions: Concepts of distribution and probability	One hour	Explain the concept of distribution and probability using partition functions
Boltzmann distribution law	One hour	Derive the Boltzmann distribution law
Interpretation of partition functions- translational and rotational	One hour	Deduce the equations for translational and rotational partition functions
vibrational and electronic partition functions	One hour	Deduce the equations for vibrational and electronic partition functions
Relationship between partition functions and thermodynamic functions (only S & G)	Two hours	Deduce the equations for relationship between partition functions and entropy and free energy.

Photochemistry –I		
Electronic transitions in molecules. The Franck Condon principle		When a molecule exposed to light then the change in electronic transitions in molecule are explain by Franck Condon prinicple
Electronically excited molecules- singlet and triplet states		Jablonski diagram explain the electronically excited molecules change in direction to develop the singlet and triplet states
Radiative life times of excited states-theoretical treatment. Measured life times		Explain the life time measurement of excited molecules.
Quantum yield and its determination. Experimental set up of a photochemical reaction		Calculate the quantum yield of a molecule the experimental set up for any photochemical reaction
Actinometry-ferrioxalate and uranyl oxalate actinometers – problems		Explain the various types of chemical actinometers and numerical are solving by using quantum yield equation.
Derivation of fluorescence and phosphorescence quantum yields		By using steady state principle deduce the quantum yield equation for fluorescence and phosphorescence
E-type delayed fluorescence- evaluation of triplet energy splitting(ΔE_{ST})		Explain the reverse intersystem crossing of molecule with very small singlet-triplet energy gap and deduce the equation.
Photophysical processes photophysical kinetics of unimolecular reactions		For unimolecular reactions alters the transition state kinetics and apply the steady state principle to deduce the equation
Calculation of rate constants of various photophysical processes-problems, State diagrams		Discuss the numerical problems for photophysical processes therough stste diagrams
Photochemical primary processes. Types of photochemical reactions		Discuss the types of photochemical reactions for a primary processes
electron transfer, photodissociation, and addition reactions with examples		Discuss the photochemical reactions such as electron transfer, photodissociation, and addition reactions with examples
abstraction, oxidation and isomerization reactions with examples		Discuss the photochemical reactions such as abstraction, oxidation and isomerization reactions with examples
Effect of light intensity on the rates of photochemical reactions.		The intensity of the light influences the rate of the photochemical reaction due to change of photo-flux
Photosensitization. Quenching-Stern-Volmer equation		Explain the photosensitization process and quenching process then deduce the Stern-Volmer equation.
Introduction to fast reactions- Principle of flash photolysis		Explain the concept of fast reaction with examples and principle of flash photolysis.

Quantum chemistry-II		
Cartesian, Polar and spherical polar coordinates and their interrelations.		Deduce the equations and explain the relationship between Cartesian, Polar and spherical polar coordinates
Schrodinger equation for the hydrogen atom- separation into three equations.		Deduce the equations for Hydrogen atom by using separable and variable method
Hydrogen like wave functions. Radial and angular functions		Similarly deduce the equations for hydrogen type systems. Discuss the graphically by Radial and angular functions.
Quantum numbers n, l and m and their importance. The radial distribution functions		Explain the significance of quantum number and radial distribution functions
Hydrogen like orbitals and their representation. Polar plots, contour plots and boundary diagrams		Plot the various functions such as polar, contour and boundary diagrams
Many electron systems. Approximate methods. The variation method-variation theorem and its proof.		Discuss the multi-electron system using approximate method such as variation method
Trial variation function and variation integral. Examples of variational calculations. Particle in a box.		Apply the variation theorem for particle in a box and correlate energy value.
Construction of trial function by the method of linear combinations.		By using two or more wave functions to construct the trial function through linear combinations
Variation parameters. Secular equations and secular determinant.		Deduce the variation parameters and secular equations and determinant for hydrogen molecule
Bonding in molecules. Molecular orbital theory-basic ideas.		Basic ideas for bonding in molecules through molecular orbital theory
Construction of MOs by LCAO, H_2^+ ion.		Construct the molecular orbitals by using LCAO for H_2^+ ion.
The variationan integral for H_2^+ ion.		Deduce the variationan integral for H_2^+ ion
Detailed calculation of Wave functions and energies for the bonding and antibonding MOs.		Detailed calculation of Wave functions and energies for the bonding and antibonding MOs for hydrogen molecule
Physical picture of bonding and antibonding wave functions. Energy diagram.		Physical picture of bonding and antibonding wave functions. Energy diagram for hydrogen molecule
The MO wave function and the energy of H2 molecule MO by LCAO method and Valence bond method (detailed calculations not required)		Discuss the MO wave function and the energy of H2 molecule MO by LCAO method and Valence bond method
Comparison of MO and VB models		Discuss the omparison of MO and VB models

Solid state chemistry & Nanoparticles and their applications		
Electronic structure of solids, Band theory, band structure of metals, insulators and semi-conductors		Explain the Electronic structure of solids, Band theory, band structure of metals, insulators and semi-conductors with examples
Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi-conductors		Explain the Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi-conductors
Photo conductivity and photovoltaic effect – p-n junctions		Discuss the photo conductivity and photovoltaic effect and p-n junction
Occurrence of superconductivity. Destruction of superconductivity by magnetic fields – Meissner effect.		Origin of superconductivity. Discuss the destruction of superconductivity by magnetic fields by Meissner effect
Types of superconductors. Theories of super conductivity – BCS theory		Explain the various types of superconductors and theories of super conductivity – BCS theory
High temperature superconductors: Structure of defect perovskites. High Tc superconductivity in cuprates		Explain the High temperature superconductors: Structure of defect perovskites. High Tc superconductivity in cuprates
Phase diagram of Y-Ba-Cu-O system. Crystal structure of $YBa_2Cu_3O_{7-x}$.		Discuss the various phases of phase diagram of Y-Ba-Cu-O system and crystal structure of $YBa_2Cu_3O_{7-x}$.
Preparation of 1-2-3 materials. Origin of high Tc superconductivity.		Explain the preparation method for 1-2-3 materials. Introduction and discuss on high Tc superconductivity
Introduction to nanoparticles. Reduced dimensionality in solids – zero dimensional systems		Discuss the nanoscience and nanotechnology, reduced dimensionality in solids and zero dimensional systems
Fullerenes, quantum dots. One dimensional systems, carbon nano tubes		Explain the structural features of Fullerenes, quantum dots. One dimensional systems and carbon nano tubes and its applications
Preparation of nano particles –top down and bottom up methods.		Discuss the method of preparation of nanoparticles through top-down and bottom-up approaches
Preparation of nanomaterials- – sol gel methods, chemical vapor deposition method and thermolysis		Discuss the preparation of nanomaterials- various methods such as sol gel methods, chemical vapor deposition method and thermolysis
Characterization of nanoparticles – experimental methods – powder X-ray diffraction		Characterization of nanoparticles – experimental methods – powder X-ray diffraction by confirmed the phase and calculate index of the system
transmission electron microscopy (TEM), and atomic force microscopy (AFM)		Morphology and particle size of the nanomaterials through TEM and surface roughness calculate by using AFM
Optical properties of nanoparticles, Applications of nanoparticles		Discuss the optical properties of nanoparticle with different sizes and its applications in photocatalysis.

NIZAM COLLEGE : DEPARTMENT OF CHEMISTRY

LESSON PLAN FOR THE ACADEMIC YEAR 2017-2018 (Semester II)

Class : M. Sc Previous **Section:** Chemistry

Course/Paper: IV- CH 204 (ANALYTICAL TECHNIQUES and SPECTROSCOPY - II)

Unit: ASP-05: **Electro and thermal Analytical Techniques** **No. of Hours Allotted**: 15

Topics to be covered	No. of Hours
Introduction to electroanalytical techniques - Types and Classification of Electro analytical Methods	1
D.C Polarography: Instrumentation - Dropping mercury electrode (diagram and explanation of each component) – working of polarograph and polarogram	2
Types of current involoved in polarography – Residual current, Migration, Limiting current,	1
Two electrode assembly -Working electrode, reference electrode. Three electrode assemble – WE, RE and Auxiliary electrode	1
Ilkovic equation and its significance – consequence of Ilkovic equation	1
Applications of polarography in qualitative and quantitative analysis – mixture analysis, application to inorganic (metal ion) and organic compounds analysis	1
Determination of stability constant – derivation	1
Brief account of (i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography – principle, model plots, and advantages over DC polarography	2
Amperometric titrations: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances like Pb^{2+}, organic compounds	1
Cyclic Voltammetry: Principle, instrumentation, Applications. Cyclic voltammetric study of insecticide parathion	1
Thermal techniques-Introduction, types of thermo analytical methods – TGA, DTA, DSC, TT, TMA, DMA, etc.	1
Thermogravimetry principle and applications of thermogravimetry – instrumentation and working	1
Differential thermal analysis- principle and applications of DTA. Differential scanning calorimetry. DSC: Principle, and application of DSC	1
	15hrs

Name of the Teacher: **Dr. S. Sree Kanth** Head, Department of Chemistry
Signature: Signature:

Unit: ASP 06: **NMR spectroscopy-II (^{1}H, ^{19}F and ^{31}P NMR)** **No. of Hours Allotted**: 15

Topics to be covered	**No. of Hours**
Introduction of NMR and recap of importants points of sem1 syllabus of NMR	1
Types of NMR spectroscopy- First order and non first order spectra, differences between first order and non first order spectra	1
Equivalent and non-equivalent protons, enantio topic and diastereotopic protons	1
Representation of NMR first order spectrum e.g., AX, AX_2,	1
Representation of NMR first order spectrum AX_3, A_2X_3, AMX	1
Representation of NMR non-first order spectrum and AB, ABC pattern	1
Methods of simplification of complex spectra: increased field strength,	1
Methods of simplification of complex spectra: deuterium exchange, Lanthanide shift reagents	1
Methods of simplification of complex spectra: double resonance techniques.	1
Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid.	1
NuclearOverhauser enhancement (NOE). Fluxional molecules bullvalene, [η5-C_5H_5M], [η5-$(C_5H_5)_2$ Ti η1-$(C_5H_5)_2$] and [η4C_8H_8Ru$(CO)_3$].	1
^{19}F NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F, ^{1}H and ^{31}P: 1,2 dichloro-1,1 difluoro ethane, BrF_5, SF_4, PF_5, ClF_3, IF_5, CF_3CH_2OH	1
^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P, ^{19}F, ^{1}H and ^{13}C: ATP, Ph_3PSe, P_4S_3, H_3PO_4, H_3PO_3, H_3PO_2, HPF_2, PF_6^-, PH3, [Rh $(PPh_3)Cl_3$] (Rh I=1/2)	1
Introduction to solid state NMR: Magic angle spinning (MAS).Applications of solid state NMR.	2
	15hrs

Name of the Teacher: **Dr. Y. Hemasri** Head, Department of Chemistry

Signature: Signature:

Unit: ASP-07: **Mass Spectroscopy** **No. of Hours Allotted**: 15

Topics to be covered	**No. of Hours**
Introduction to Mass spectra. Application. Principles of mass spectrometer.	1
Definitions- Molecular ion , Charge to mass ratio, Representation.Fragment ion / daughter ion., Base peak. Bar graph, tabular column	1
Bond Fissions - Homolysis, Hemi- heterolysis – eg – Methane.	1
Types of fragments-classification. Positive ions, Neutral species, odd electron species, even electron species, - Fragmentation pattern	1
Even electron Rule. Stability. Nitrogen Rule- Fragmentation pattern with two examples.	1
Isotopic peaks – relative percentage- natural abundance.	1
Importance of Isotopic peaks- Discussion with (m+1) & (m+2) peaks	1
Determination of Molecular formula – Guidelines – problems	1
Problems contd.	1
Meta stable ion peaks- Fragmentation pattern- α cleavage.	1
β- cleavage- allylic, Benzylic and vinylic	1
RDA fragmentation- Mc lafferty Fragmentation	1
Ortho effect- principles of EI, CI, FAB mass.	1
Principles of SIMS , MALDI	1
Principles of GC-MS & LC-MS	1
	15hrs

Name of the Teacher: **Dr. P. Sarita Rajender** Head, Department of Chemistry

Signature: Signature:

Unit: ASP-08: **Photoelectron & ESR spectroscopy** **No. of Hours Allotted**: 15

Topics to be covered	No. of Hours
Photoelectron Spectroscopy – Introduction to electron spectroscopy, photoionization, photoemission, principle; types of PES – X-ray Photoelectron spectroscopy (XPS) and Ultraviolet Photoelectron Spectroscopy (UPS)	1
Basic instrumentation of PES – schematic diagram, terms like Ionization potential, , Kinetic energy, Binding energy of electron	1
Koopmans' Theorem: Ionization energy – types of ionization energies – vertical and adiabatic ionization energies, relation between ionization energies and molecular orbitals.	1
X-ray photoelectron spectroscopy (XPS/ESCA): Principle, instrumentation, working of electrospectrophotometer, ESCA in qualitative analysis, chemical shifts.	1
UPS – principle, instrumentation, sources used, working of the instrument, applications of UPS	1
Auger Electron Spectroscopy: Principle, Auger electron, instrumentation, comparison of XPS with AES, applications of Auger electron spectroscopy.	1
Photoelectron spectra of simple molecules – N_2, CO, O_2, F_2,– structures of PES bands, potential energy curves	1
PES of HF, NH_3, H_2O - structures of OES bands and potential energy curves.	1
Interpretation of vibrational spectral data for ionized (M^+)species; prediction of nature of molecular orbitals.	1
Electron Spin Resonance (ESR) – Principle of ESR, comparison with NMR, Instrumentation, selection rules.	1
Hyperfine and super hyperfine splitting, interpretation of Lande's 'g' factor, isotropy and anisotropy in 'g' vales, Hyperfine coupling constant.	1
Zero-field splitting, Kramer's degeneracy, Quadrapolar interactions.	1
Study of free radicals and transition metal complexes – ESR spectra and interpretation.	1
Covalency of complexes – Cu (II) Bissalcylaldimine, Bis-acetylacetanato vanadyl (II) and Hexachloro iridium (IV) complexes.	1
Discussion of PES and ESR.	1
	15hrs

Name of the Teacher: **Dr. B.Sireesha**
Signature:

Head, Department of Chemistry
Signature: