NATIONAL COLLEGE (AUTONOMOUS), TIRUCHIRAPALLI – 1

M.Sc., Chemistry – Course Structure under CBCS

(Applicable to the candidates admitted from the academic year 2013-2014 onwards)

Semester	Paper No.	Title of the Paper	Instr Hrs/ Week	Credit	Exam Hrs.	Marks			Total
						Internal	External		
							W	O	
I	**CC I**	INORGANIC CHEMISTRY-I	6	5	3	25	75		100
	CC II	ORGANIC CHEMISTRY-I	6	5	3	25	75		100
	CC III	INORGANIC CHEMISTRY (PRACTICALS	6	5	3	25	75		100
	CC IV	ORGANIC CHEMISTRY PRACTICALS)	6	5	4	25	70	5	100
	EC I	ANALYTICAL AND COMPUTER APPLICATION IN CHEMISTRY	6	4	3	25	75		100
		Total	**30**	**24**					**500**
II	**CC V**	PHYSICAL CHEMISTRY-I	6	5	3	25	75		100
	CC VI	INORGANIC CHEMISTRY-II	6	5	3	25	75		100
	CC VII	INORGANIC CHEMISTRY (PRACTICALS)	6	5	3	25	75		100
	CC VIII	ORGANIC CHEMISTRY (PRACTICALS)	6	5	4	25	70	5	100
	EC II	GREEN AND ENVIROMENTAL CHEMISTRY	6	4	3	25	75		100
		Total	**30**	**24**					**500**
III	**CC IX**	ORGANIC CHEMISTRY-II	6	5	3	25	75		100
	CC X	PHYSICAL CHEMISTRY-II	6	5	3	25	75		100
	CC XI	PHYSICAL CHEMISTRY (PRACTICALS)	6	5	4	25	70	5	100
	EC III	PHYSICAL METHODS IN INORGANIC CHEMISTRY	6	4	3	25	75		100
	EC IV	NANO MATETIALS AND SYNTHEIC ORGANIC CHEMISTRY	6	4	3	25	75		100
		Total	**30**	**23**					**500**
IV	**CC XII**	ORGANIC CHEMISTRY-III	6	5	3	25	75		100
	CC XIII	PHYSICAL CHEMISTRY (PRACTICALS-II)	6	5	4	25	70	5	100
	EC V	PHYSICAL CHEMISTRY-III	6	4	3	25	75		100
		Project (Dissertation 75 marks & Viva Voice – 25 Marks)	**12**	**5**	**-**	**75**	**-**	**25**	**100**
		Total	**30**	**19**					**400**
				90					**1900**

There will be oral test for all practical examinations. The oral test will carry 5 marks in the external component

INORGANIC CHEMISTRY I - P13CH1

Semester : I **Core Course: I**

Instruction Hours/Week: 6 **Credit: 5**

UNIT I: Boron, Sulphur, Nitrogen and Phosphorus Compounds

Chemistry of boron - carboranes - metallocarboranes - importance of icosahedral frame work of boron atoms in boron chemistry - closo, nido and arachno structure - structural study by Wade's rule. S-N compounds - S_4N_4, S_2N_2, polythiazyl S_xN_4 compounds - S-N cations and anions. S-P compounds - molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}.

UNIT II: Ionic Model

Lattice energy - Born-Lande equation - Kapustinski's equation - High-Tc superconductors - solid-state reactions - types and example.

UNIT III: Crystalline State

Crystal systems and lattice types - Bravais lattices - crystal symmetry - point groups and space groups (No detailed study) - Miller indices - reciprocal lattice concept - close packed structures - BCC, FCC, HCP - voids - coordination numbers - crystal binding - molecular, covalent, metallic and hydrogen bonded crystals.X-ray diffraction by crystals - function of crystals - transmission grating and reflection grating - Bragg's equation - diffraction methods - powder, rotating crystal, oscillation and Weisenberg methods - indexing and determination of lattice types - unit cell dimensions of cubic crystals - structure factor - Fourier synthesis.

UNIT IV: Inorganic Photochemistry

Electronic transitions in metal complexes - metal centered and charge transfer transitions - various photophysical and photochemical processes of coordination compounds - unimolecular charge-transfer photochemistry of cobalt(III) complexes - mechanism of CTTM photoreduction.Ligand field photochemistry of Cr(III) complexes - Adamson's rule - photoactive excited states - V-C model - photophysics and photochemistry of Ru-polypyridine complexes - emission and redox properties - photochemistry of organometallic compounds - metal-carbonyl compounds - compounds with metal-metal bonding - Reinecke's salt - chemical actinometer.

UNIT V: Supramolecular Chemistry

Concepts and languages of supramolecular chemistry - hydrogen bonds - C-H...X interactions - halogen bonds - - interactions - non-bonded interactions.

M.O.F. (Metallo Organic Frameworks) - organometallic systems - combination of different interactions to design molecular rods, triangles ladders, networks etc - design of nanoporous solids - supramolecular metallocatalysis - cocatalysts - catalysis of synthetic reactions - biomolecular and abiotic catalysts - role of supramolecular chemistry in the development of nanoscience and technology - supramolecular devices - supramolecular photochemistry.

References:

01. M. C. Day and J. Selbin,"Theoretical Inorganic Chemistry",2nd Edition, 1985, Affiliated East-West Press Pvt. Ltd, New Delhi.
02. J. E. Huheey, E. A. Keiter and R. L. Keiter, "Inorganic Chemistry – Principles of Structure and Reactivity", Harper Collins College Publishers, 4th Edition, 1993.
03. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry" 5th Edition, Wiley-Interscience Publication, New York, 1988.
04. L. W. Azaroff, "Introduction to Solids", Mc-Graw Hill.
05. N. B. Hannay, "Solid State Chemistry", Printice Hall, New Delhi, 1976.
06. F. C. Philips, "An Introduction to Crystallography", Longman.
07. K. F. Purcel and J. C. Kotz, Inorganic Chemistry", W. G. Saunder's Company, Philadelphia.
08. Shriver, Atkins and Langford, "Inorganic Chemistry", ELBS.
09. J.Ferraudi, "Elements of Inorganic Photochemistry" , Wiley, New York, 1988.
10. A. W. Adamson and P. D. Fleischauer, "Concepts of Inorganic Photochemistry, Wiley, New York, 1975.
11. J. L. Atwood and J. W. Steed, "Supramolecular Chemistry: A concise Introduction", John Wiley & Sons, 2000.
12. J. M. Lehn, "Supramolecular Chemistry: Concepts and Perspectives", Wiley-. VCH, 1995.

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ORGANIC CHEMISTRY I - P13CH2

Semester : I **Core Course: II**

Instruction Hours/Week: 6 **Credit: 5**

UNIT I: Nomenclature of Organic Compounds

Nomenclature - aromatic and hetero aromatic systems - Nomenclature of heterocyclics having not more than two hetero atoms such as oxygen, nitrogen and sulphur - Nomenclature of heterocyclic compounds of fused ring system - Nomenclature of alicyclic, bicyclic and tricyclic compounds. **Reactive Intermediates:** Classical and non-classical carbocations, carbanions-free radicals, carbenes, nitrenes and arynes - general methods of generation, detection and reactivity of these intermediates. **Electronic Effects:** Inductive effect - resonance effect - hyperconjugation (Baker-Nathan effect) hydrogen bonding (inter and intramolecular)

UNIT II: Organic Stereochemistry - I

Optical isomerism - Optical activity and chirality - elements of symmetry - stereochemistry of overcrowded molecules (hexahelicene, ansa compounds, cyclophanes and trans cycloalkenes - Newmann, Sawhorse and Fischer projections - representation and

interconversion - Absolute configuration - R&S notations for special molecules (allenes, spirans, biphenyls) R-S nomenclature of cyclic chiral compounds - molecules with more than one chiral center. Asymmetric synthesis - Cram's rule and Prelog's rule- Optical purity - determination of enantiomeric excess by NMR - definition of terms like prochirality, enantiotopic and diastereotopic atoms, groups and faces - stereoselective and stereospecific reactions.

UNIT III: Organic Stereochemistry - II

Geometrical isomerism: E, Z - determination of configuraton of geometrical isomers (cyclisation, converting into compounds of known configuration, dipolemoment, converting into less symmetric compounds - spectroscopic methods) configuration of cyclic and bicyclic ring systems - cis-trans nomenclature of three, four and six membered substituted cyclic systems - decalins. **Dynamic Stereochemistry:** Quantitative correlation between conformation and reactivity - Winstein-Eliel equation - Curtin Hammet principle - saponification of an ester - esterification of an alcohol - chromic acid oxidation of cyclohexanols - neighbouring group participation - deamination of 2-amino cyclohexanol.

UNIT IV : Methods of Determining Reaction Mechanisms

Kinetics and non-kinetic methods of determination of reaction mechanisms - Thermodynamic and kinetic aspects of organic reactions ,energy profile diagrams - spectroscopic studies, isotopic effects - intermediate versus transition states - product analysis and its importance - crossover experiments - isotopic labelling studies. **Correlation Analysis:** Linear Free Energy Relations - Hammet equation - significance - sigma and rho applications and limitations - Taft, Swain-Scott-Grunwald-Winstein equations and their applications, classification of solvents.

UNIT V: Natural Products

Carbohydrates: Polysaccharides - structure of starch and cellulose, configuration of carbohydrates – photosynthesis. **Antibiotics:** Chemotherapy - definition LD_{50} - Structural elucidation and synthesis of penicillin, streptomycin - cephalosporin-C. **Steroids:** Classification - structural elucidation of cholestrol (synthesis not required), structural elucidation and synthesis of Vitamin D, estrone, progestrone, ergosterol, androsterone and equilenin - Classification and functions of prostaglandins

References:

01. R. Panico, W. H. Powell, L. Jean. C. Richer, “A guide to IUPAC Nomenclature of Organic Compounds”, (1993), Jain Interscience.

02. S. C. Pal, “Nomenclature of Organic Compounds”, (2008), Narosa Publishing House.

03. Jerry March, “Advanced Organic Chemistry: Reactions, Mechanisms and Structure”, 5th Edition, Wiley (2000).

04. D. Nasipuri, "Stereochemistry of Organic Compounds-Principles and Applications", 2nd Edition, New Age International (2002).
05. P. S. Kalsi, "Stereochemistry", Wiley Eastern Ltd, 1990.
06. E. L. Eliel and S. H. Wilen, "Stereochemistry of Organic Compounds", John Wiley, 2003.
07. T. H. Lowry and K. S. Richardson, "Mechanism and Theory in Organic Chemistry", 2nd Edition, Harper and Row, 1981.
08. O. P. Agarwal, "Chemistry of Organic Natural Products", Volume I & II, Goel Publishers, 1997.
09. I. L. Finar, "Organic Chemistry", Volume-II, 5th Edition (1975).

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INORGANIC CHEMISTRY PRACTICAL I - P13CH3P

Semester : I&II **Core Course : III**

Instruction Hours/Week: 6 **Credit: 5**

Semi-micro qualitative analysis of a mixture containing two common and two rare cations. Estimation of Copper, Ferric, Nickel, Chromium and Manganese using photoelectric colorimeter.

References:

01. A. I. Vogel, "Quantitative Inorganic Analysis", ELBS, 3rd Edition, 1971.
02. V. V. Ramanujam, "Inorganic Semimicro Qualitative Analysis", The National Publishing Company, Madras, 1974.

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ORGANIC CHEMISTRY PRACTICAL – I – P13CH4P

Semester : I &II **Core Course : IV**

Instruction Hours/Week: 6 **Credit: 5**

Qualitative Analysis of an Organic Mixture Containing Two Components

Pilot separation, bulk separation, analysis, derivatization.

Preparation of Organic Compounds (Single Stage)

(a) Methyl-m-nitrobenzene from methyl benzoate (nitration)

(b) Glucose penta acetate from glucose (acetylation)

(c) Resacetophenonone from resorcinol (acetylation)

(d) Phenyl-azo-2-naphthol from aniline (diazotization)

(e) -Naphthylmethylether from -Naphthol (methylation)

(f) Dibenzalacetone from benzaldehyde

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ANALYTICAL AND COMPUTER APPLICATIONS IN CHEMISTRY - P13CH5E

Semester : I **Elective Course: I**

Instruction Hours/Week: 6 **Credit: 4**

UNIT I: Error Analysis and Instrumental Methods of Analysis

Various types of Error - accuracy Precision, significant figures - Standard deviation - Correlation and regression - Fitting of linear equations - Multiple linear regression analysis. Principles and Applications of Extended X-ray absorption fine structure (EXAFS) - Atomic Absorption Spectroscopy (AAS) - Flame Emission Spectroscopy (FES).

UNIT II: Chromatography

Solvent extraction - Principles of ion exchange, paper, thin layer and column Chromatography techniques - Columns, adsorbents, methods, R_f values, McReynold's constants and their uses - HPLC techniques - Adsorbents, Columns, detection methods, estimations, preparative column - GC-MS techniques : methods, principles and uses.

UNIT III: Thermoanalytical Methods and Fluorescence Spectroscopy

Principles and application of Thermogravimetry Analysis (TGA) Differential Thermal Analysis (DTA). Differential Scanning Calorimetry (DSC). Thermometric titrations.Basic aspects of synchronous fluoresence spectroscopy - Flow cytometry - Instrumentation on fluorescence ratio - Fluorimeters (quantization)- applications.

UNIT IV: Computer Applications in Chemistry

Introduction to computers and computing - Block diagram of a PC and the functions of the various units of computer - High and low level languages - Introduction to net working - LAN, WAN, Internet and Intranet - WorldWideWeb - ChemWeb - E-journals - search engines for chemistry.

Introduction to C language - Structure of C program - Control statements – 01. Loops - recursion. Examples of simple chemistry Programmes.

02. Conversion of Celsius temperature to Kelvin temperature

03. Applications of Beer-Lambert Law.

04. Linear least square - Fit log k vs I/T plot to get Arrhenius parameters.

05. Determination of Anharmonicity constant and dissociation energy calculation.

UNIT V: Molecular Modelling Basics

Molecular modeling - Coordinate systems - Cartesian and internal coordinate systems - bond lengths, bond angles and torsion angles - distance matrix - stick models - space filling models - potential energy surfaces - Molecular mechanics - application and parameterization - advantages and limitations of force fields.

References:

01. R. Stock and C. B. F. Rice, Chromatographic Methods, Chapman and Hall,New York.

02. V. K. Srivastava and K. K. Srivastava, Introduction to Chromatography, S. Chand & Co., New Delhi, 2nd ed, 1981.

03. Willard, Merrit, Dean and Settle, Instrumental methods of Analysis CBS Publishers and Distributors, 6th ed., 1986.

04. Skoog, D. A. West, D. M. Holler. P. J. Fundamentals of Analytical Chemistry, 7th edition, Harcourt College Publishers, Singapore. (Page 523-665).

05. A. Sharma, S. G. Schulman, Introduction to Fluorescence Spectroscopy. Wiley-Interscience, New York, 1999.

06. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th ed. Tata Mc.Grw –Hill, New Delhi,1994.

07. Vogel, A.I. Text Book of Quantitative Inorganic Analysis, ELBS.

08. E. Balaguruswamy, "Programming in ANSI C", Tata McGraw Hill, 2nd Edition, NewDelhi, 1999.

09. S. K. Basandra, "Local Area Networking",.Galgotia, New Delhi, 1999.

10. A. S. Tanenbaum, "Computer Networks". Prentice Hall of India, 1996.

11. S. M. Bachrach, " Internet for Chemists", ACS Publications. Washigton, DC,1996.

12. A. R. Leach, " Molecular Modelling Principles and Applications", 2nd Edition, Prentice Hall, 2001.

13. W. B. Smith, "Introduction to Theoretical Organic Chemistry and Molecular Modelling" John Wiley, New York, 1996.

14. Tim Clark, "A Handbook of Computational Chemistry", John Wiley, New York, 1985

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PHYSICAL CHEMISTRY I - P13CH6

Semester : II **Core Course: V**

Instruction Hours/Week: 6 **Credit: 5**

UNIT I: Quantum Chemistry

Inadequacy of classical mechanics - Black body radiation, Planck's concept, - Wave - particle dualism - Uncertainty Principle Conservation laws - Lagrangian and Hamiltonian equations of motions - Inadequacy of old quantum theory.Schrodinger equation - Postulatory basis of quantum mechanics - Operator algebra: operator, linear and hermitian, eigen functions and eigen values, angular momentum operator, commutation relations.Application of wave mechanics to simple systems - particle in a box, one- and three-dimensional - distortion of the box and Jahn-Teller effect - quantum numbers - Orthogonalisation and normalization – Potential barrier of definite thickness: Quantum mechanical tunnelling

UNIT II: Molecular Spectroscopy - I

Einstein coefficient of absorption and transition probabilities - basis of selection rules - Representation of spectra - the width and intensity of spectra transitions oscillator strength.

Electronic spectra - electronic spectra of molecules - Born Oppenheimer approximation - vibrational coarse structure - Franck-condon principle - dissociation energy - fortrat diagram - Pre-dissociation - various types of transitions - solvent effect on spectra.

Infra red spectra - vibrational spectra - selection rules - harmonic and anharmonic oscillators - vibration and rotation spectra of diatomic molecules - vibration spectra of polyatomic molecules - normal vibration and normal coordinates - Influence of rotation on the spectra of polyatomic molecules - parallel and perpendicular bands - FTIR.Laser Raman spectra - rotational Raman spectra of linear molecules - vibrational Raman spectra - rotational fine structure - Fermi resonance.

UNIT III: Classical Thermodynamics

Thermodynamics of systems of variable composition - relationship between partial molar quantities - Gibbs-Duhem equation and its applications - determination of chemical potential - variation of chemical potential with temperature and pressure.

Thermodynamic properties of real gases - Fugacity - definition - methods of determination of fugacity - variation of fugacity with temperature and pressure - activity and activity coefficient - definition - Standard states for gases, liquids, solids and component of solutions - determination of activity and activity coefficient from freezing point - EMF and solubility measurements.

Phase rule - Application of phase rule to the three component systems - systems of three liquids - solid-liquid system (Eutectic systems - two salts and water).

UNIT IV: Chemical Kinetics

Theories of reaction rate - Absolute reaction rate theory (ARRT) - significance of reaction coordinate - Potential energy surfaces - Kinetic isotopic effect - molecular dynamics - Marcus theory of electron transfer processes - Principle of microscopic reversibility - Steady-state approximation.Chain reactions - thermal and photochemical reactions between hydrogen and halogens - explosions and hydrogen - oxygen reactions.Factors influencing reaction rates in solution - application of ARRT to solution kinetics - effect of solvent and ionic strength, influence of pressure on rates in solution - significance of volume of activation.

Acid-base catalysis - Hammett's acidity function - Bronsted relation LFER - Hammett and Taft equations.

UNIT V: Surface Phenomena

Adsorption and free energy reaction at interphase - potential energy diagram - Lennard-Jones plot - surface area determination - heats of adsorption - determination - adsorption from solution - Gibbs adsorption theorem - solid-liquid interface - Wetting and contact angle - solid-gas interfaces - soluble and insoluble films.Surface tension: methods of measuring surface tension - electrical phenomena at interface including electro kinetic phenomenon - Micelles and reverse micelles - solubilisation - micro emulsion or micellar emulsions.Role of surface in catalysis: semiconductor catalysis - n- and p-type surfaces - kinetics of surface reaction involving adsorbed species. Langmuir-Hinshelwood mechanism of bimolecular reaction - Langmuir-Rideal mechanism - Rideal-Eley mechanism.

References:

01. A. K. Chandra, Introductory Quantum Chemistry, 4th ed., Tata McGraw Hill, 1994.

02. R. K. Prasad, Quantum Chemistry, 2nd ed., New Age International Publishes (2000), UNIT I

03. I. N. Levine, Quantum Chemistry, 4th ed., Prentice Hall of India Pvt Ltd., (1994), UNIT I

04. D. A. McQuarrie, Quantum Chemistry, University Science Books (1998), UNIT I

05. S. Glasstone, Introduction to Theoretical Chemistry, Affiliated East-West Press UNIT I & II

06. G. N. Barrow, Introduction to Molecular Spectroscopy, International Mc.Graw Hill Edition (1993), UNIT II

07. G. N. Barrow, Introduction to Molecular Spectroscopy, International McGraw Hill Student Edition (1984), UNIT II

08. B. P. Straughan and S. Walker, Spectroscopy, Vol.I to III, Chapman Hall, London (1976), UNIT II

09. S. Glasstone, Thermodynamics for Chemists, East-west Affiliated Pvt Ltd, New Delhi (1969), UNIT III

10. R. P. Rastogi and R. R. Misra, An Introduction to Chemical Thermodynamics Vikas Publishing House Pvt Ltd., (1992), UNIT III

11. Kloz and P. M. Rosenberg, Chemiscal Thermodynamics: Basics Theory and Methods, 3rd ed., W. A. Benjamin, NY (1974), UNIT III

12. K. J. Laidler, Chemical Kinetics,2nd ed, Tata McGraw Hill (1975),UNITIV

13. A. A. Frost and R. G. Pearson, Kinetics and Mechanisms, John Wiley & Sons (1953), UNIT IV

14. J. C. Kuriacose and J. Rajaram, Kinetics and Mechanisms Transformations, Macmillan & Co., (1993), UNIT IV

15. P. W. Atkins, Advanced Physical Chemistry, 7th ed., Clarendon (2002) UNIT V

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INORGANIC CHEMISTRY II - P13CH7

Semester : II **Core Course : VI**

Instruction Hours/Week: 6 **Credit: 5**

UNIT I: Coordination Chemistry Principles

Nomenclature of mono and polynuclear coordination compounds - valence bond theory - formation of octahedral complexes on the basis of VBT - limitations of VBT - crystal field theory (CFT) - shapes of d-orbitals in octahedral symmetry - CFSE - strong field and weak field splitting - calculation of CFSE - splitting in tetrahedral symmetry - only weak field - tetragonal symmetry - differences between tetrahedral and tetragonal symmetry - Jahn-Teller distortions - splitting pattern in various symmetries - factors affecting the magnitude of splitting (10 Dq) - spectrochemical series - Jorgenson's relation - evidences for CFT - magnetism and colour of transition metal ions - LFT.

MO theory - octahedral, tetrahedral and square-planar complexes - -bonding and MO theory - ligands having filled and empty -bonds - effect of 10 Dq - evidences for - bonding from X-ray crystallography, IR and photoelectron spectroscopy - nephelauxetic effect.

UNIT II: Coordination Chemistry and Reaction Mechanisms

Stability of coordination compounds - detection of complex formation in solution - stability constants - step-wise and overall formation constants - pH metric, and photometric methods of determination of formation constants - factors affecting stability - statistical and chelate effects - forced configuration.

Kinetics and mechanism of reactions - labile and inert complexes - ligand displacement reactions - hydrolysis and anation reactions in octahedral and square planar complexes - trans effect - theory and applications - electron transfer reactions - complementary and non complementary types - inner sphere and outer sphere processes - isomerisation and racemisation - reactions of coordinated ligands - template effects - synthesis of macrocyclic ligands.

UNIT III: Bioinorganic Chemistry

Biological role of metal ions - nucleation and crystal growth of various biominearls such as calcium phosphate, calcium carbonate and iron biominearls - characterization of K^+, Na^+, Ca^{2+} and Mg^{2+} complexes of alkali and alkaline earth metal ions with macrocycles - ion channels - ion pumps.Oxygen transport (Hb and Mb) and storage - carbonic anhydrase - carboxypeptidases - iron-sulphur proteins and non-heme iron cytochromes of electron transport chain - cytochrome P-450 enzymes - coenzyme B12 - nitrogen fixation - porphyrin ring system - chrlorophyll - photosynthesis - synthetic model.

UNIT IV: Organometallic Reactions

Ligand association and dissociation reactions-oxidative addition and reductive elimination reactions.Hapticity - ligand classification - synthesis and structure - uses of typical organometallics in organic synthesis - such as metal alloys and organometallic hydrides.Metal carbenes - carbynes - carbonylate anions - metal clusters.Complexes of -acceptor ligands - carbonyls - 18 electron rule - applications and limitations - isolobal concept - applications to structure of carbonyls - carbonyl hydrides - nitrosyl complexes - bridging and terminal nitrosyls - bent and linear nitrosyls - dinitrogen complexes - dioxygen complexes - metallocenes - reactions - arene complexes.

UNIT V: Reaction and Catalysis by Organometallic Compounds

Catalysis by organometallic compounds - hydrogenation of olefins - hydroformylation of olefins - oxidation of olefins to aldehydes and ketones - polymerization of alkenes - cyclo oligomerisation of acetylene - Fischer-Tropsch synthesis - epoxidation - meta thesis - carbonylation of methanol.

References:

01. J. E. Huheey, E. A. Keiter and R. L. Keiter, "Inorganic Chemistry – Principles of Structure and Reactivity", Harper Collins College Publishers, 4th Edition, 1993.

02. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry" 5th Edition, Wiley-Interscience Publication, New York, 1988.

03. F. A. Kettle, "Physical Inorganic Chemistry - A Coordination Approach", Spectrum Academic Publishers, Oxford University Press, 1996.

04. P. Powell, Principles of Organometallic Chemistry", 2nd Edition, Chapman and Hall, London.

05. K. F. Purcel and J. C. Kotz, Inorganic Chemistry", W. G. Saunder's Company, Philadelphia.

06. W. U. Malik, G. P. Tuli and R. D. Madan, "Selected Topics in Inorganic Chemistry", 6th Edition, 2001, S. Chand & Company Ltd., New Delhi.

07. Gurdeep Raj, "Advanced Inorganic Chemistry", Vol. II, 8th Edition, 2002, Goel Publishing House, Meerut.

08. W. Kaim and B. Schewederski, "Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life", John-Wiley and sons, New York.

09. S. J. Lippard and J. M. Berg, "Principle of Bioinorganic Chemistry", Parima Publishing Company, New Delhi.

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INORGANIC CHEMISTRY PRACTICAL II – P13CH8

Semester : II **Core Course: VII**

Instruction Hours/Week: 6 **Credit: 5**

Titrimetry (V) and Gravimetry (G)

A mixture of solution(s) should be given for estimation

Cu (V) and Ni (G)

Cu (V) and Zn (G)

Fe (V) and Zn (G)

Fe (V) and Ni (G)

Zn (V) and Cu (G)

Preparation of the following compounds

a. Tetramminecopper (II) sulphate.

b. Potassium trioxalatochromate (III).

c. Potassium trioxalatoaluminate (III).

d. Trithioureacopper (I) chloride.

e. Trithioureacopper (I) sulphate.

Reference:

01. A. I. Vogel, "Quantitative Inorganic Analysis", ELBS, 3rd Edition, 1971.

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ORGANIC CHEMISTRY PRACTICAL II – P13CH9P

Semester : II **Core Course: VIII**

Instruction Hours/Week: 6 **Credit: 5**

Qualitative analysis of Organic Compounds

Estimation of phenol, aniline, ketone, glucose

Preparation of Organic Compounds (Double Stage)

(a) p-bromo acetanilide from aniline (acetylation and bromination)

(b) acetyl salicylic acid from methyl salicylate (hydrolysis and acetylation)

(c) 1,3,5-tribromobenzene from aniline (bromination, diazotization and hydrolysation)

(d) p-nitroaniline from acetanilide (nitrogen and hydrolysis)

(e) benzilic acid from benzoin (rearrangement)

(f) benzanilide from benzophenone (rearrangement)

(g) p-bromoaniline from acetanilide (bromination and hydrolysis)

(h) m-nitroaniline from nitrobenzene

(i) 1,2,4-triacetoxy benzene from hydroquinone (oxidation and acylation)

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GREEN AND ENVIRONMENTAL CHEMISTRY - P13CH10E

Semester : II **Elective Course: II**

Instruction Hours/Week: 6 **Credit: 4**

UNIT I: Introduction to Green Chemistry

Green chemistry - Introduction - need for green chemistry - goals of green chemistry - Anastas' twelve principles of green chemistry - Designing a green synthesis(tools) - choice of starting materials, solvents, catalysts, reagents, processes with suitable examples.

UNIT II: Microwave and Ultrasound Assisted Organic Synthesis and Biocatalysts

Microwave activation - advantages of microwave exposure - Microwave assisted reactions, condensation reactions - oxidation, reduction reactions, multicomponent reactions. **Sonochemistry** - use of ultrasound in organic synthesis(alternate source of energy) - saponification - substitution, addition, oxidation reactions, reductions. **Biocatalysts** in green synthesis - use of biocatalysts in green chemistry - advantages - biochemical (microbial) oxidation and reduction reactions - Bakers yeast mediated bio-transformation - biocatalyst mediated Baeyer-Villiger reaction.

UNIT III: Ionic liquids - Phase Transfer Catalyst and Supercritical CO_2 in Green Synthesis

Ionic liquids - synthesis, physical properties of ionic liquids - applications in alkylation, epoxidation, Friedal-Crafts reaction - Diels-Alder reactions - Knoevengal condensations and Wittig reactions. **PTC** - Definition - advantages, types of PTC reactions - synthesis of PTC, applications of PTC in organic synthesis - Michael reaction - alkylation of aldehydes and ketones. Wittig, generation of dihalocarbene, elimination reaction. **Supercritical CO_2** - phase diagram - uses in extracting natural products, dry cleaning, bromination, Kolbe-Schmidt synthesis - Friedel-crafts reaction.

Dimethyl carbonate as a methylating agent in green synthesis.

UNIT IV: Pollution from Agriculture

Pesticides - General aspects of classification in terms of chemical nature and generation wise. Mode of action of insecticides - General aspects. Bio-accumulation and bio-magnification of pesticides - Fate of insecticides in environment and environmental hazards - Major disasters with pesticides and herbicides - Toxicity of DDT, gammexene and malathion - comparison of organochlorine, organophosphate and carbamate insecticides - Detoxification

of pesticides and allied chemicals - Safer pesticides - IPM - Environmental hazards arising from fertilisers - Minimisation of environmental problems caused by fertilisers.

UNIT V: Radioactive Pollution

Nature of radioactive emission - units - Radiation from natural sources and Man-made activities - Effects of radiation on human health - Permissible radiation dose - Comparative risk analysis of fossil fuel based power generation versus nuclear power generation - Radioactive fall out - Nuclear winter: atmospheric turbidity and effects - Radioactive pollution in land, atmosphere and water - Nuclear waste disposal: Nature, general principles and strategies - Causes and prevention of nuclear reactor accidents - Chernobyl disaster - Three Mile Island disaster.

References:

01. Paul T. Anastas and John C. Warner, "Green Chemistry", Oxford University Press, Indian Edition, 2008.
02. V. K. Ahluwalia and M. Kidwai, "New Trends in Chemistry", Anamaya Publishers, 2nd Edition, 2007.
03. V. Kumar, "An Introduction to Green Chemistry", Vishal Publishers, 1st Edition, 2007.
04. V. K. Ahluwalia and R. S. Varma, "Green Solvents", Narosa Publishing, 1st Edition, 2009.
05. V.K.Ahluwalia and Renu Aggarwal, "Organic Synthetic Special Techniques", Narosa, 2nd Edition, 2009.
06. V. K. Ahluwalia, "Green Chemistry - Environmentally Benign Reactions", Ane books, India, 2006.
07. Rashmi Sanghi and N. M. Srivastava, "Environment Friendly Alternatives", Narosa Publishing House, 2003.
08. D. K. Asthana and Meera Asthana, "Environment - Problems and Solutions", S.Chand & Co Ltd.
09. Benny Joseph, "Environmental Studies", Tata McGraw Hill Publishing Company Ltd, New Delhi.

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ORGANIC CHEMISTRY II – P13CH11

Semester : III **Core Course: IX**

Instruction Hours/Week: 6 **Credit: 5**

UNIT I: Aliphatic Nucleophilic Subsitution, Aromatic Nucleophilic Subsitution and Aliphatic Electrophilic Subsitution

SN^1, SN^2, SN^i mechanisms - stereochemical factors - effect of substrate structure, leaving group, attacking nucleophile and solvent - neighbouring group participation -

substitution at allylic and vinylic carbons - ambident nucleophiles. SN^1, SNAr, Benzyne mechanisms - orientation effect of substrate structure, leaving group, attacking nucleophile.SE^1, SE^2, SE^i, mechanisms - stark enamine reaction - decarboxylation of aliphatic acids - halogenation of aldehydes and ketones.

UNIT II:Aromatic Electrophilic Substitution and Aromaticity

Arenium ion mechanism - orientation and reactivity energy profile diagrams - the ipso attack - ortho/para ratio - substitution in thiophene - pyridine.

Concept of aromaticity - Huckel's rule and Craig's rule - effect of aromaticity on bond length, ring current - non-benzenoid aromatic compounds - aromatic character in three, five, seven and eight membered rings - anti aromaticity - system with 4, 8, 10π electrons - annulene - sydnones - alternant and non-alternant hydrocarbons.

UNIT III: Addition Reactions and Addition to Carbonyl Groups

Addition to carbon - carbon multiple bonds - electrophilic addition, nucleophilic and free radical additions - orientation and reactivity - birch reduction - hydroxylation - hydroboration - epoxidation - diels Alder reaction. Michael addition - ozonolysis, Clemmenson and Wolf-Kishner reductions. Mannich, Sobbe, Benzoin, Oppenauer oxidation - MPV reduction, Darzens Glycidic esters - Grignard reagents 1,2 and 1,4 addition - Gilman reagents - Wittig reaction.

UNIT IV: Rearrangements and Elimination Reactions

Classification - mechanisms of the following rearrangements - Wagner, Meervein, Dienone-phenol, Wolff, Favorski, Steven, Sommelet Hauser, Demjenov, Von-Richer, Schmidt, Pummerer rearrangements. Mechanisms of E^1, E^2, E^1CB - stereochemistry of elimination - competition between elimination and substitution pyrolytic cis elimination - chugaev reaction - dehydration - dehydrohalogenation - hofmann degradation - cope elimination, Bredt's rule with examples.

UNIT V: Proteins, Nucleic Acids and Heterocyclic Compounds

Proteins classification - 1^0, 2^0, 3^0 and quaternary structure of proteins - denaturation of proteins - biosynthesis of proteins.Nucleotides and Nucleosides - DNA - 1^0 and 2^0 structure - replication of DNA - RNA (mRNA, tRNA and r-RNA) genes - genetic code and informational theory - determinatin of base sequence of DNA - polymerase chain reactions.Synthesis and reactions of pyrazoles, oxazoles, thiazole, imidazole, pyridazine, pyrimidine and pyrazines.

References:

01. Advanced Organic Chemistry (Reactions, Mechanisms and Structure), Jerry March - Wiley, 2001.

02. Mechanism and Structure in Organic Chemistry - Edwin S. Gould, New York, 1959.

03. Mechanism and Theory in Organic Chemistry - Thomas H. Lowry and K. S. Richardson - Addisson-Wesley, 1988.

04. Organic Reaction Mechanism - V. K. Ahluwalia and R. K. Parashar Narosa, 2002.

05. Heterocyclic Chemistry (Synthesis, Reactions and Mechanism), Raj K. Bansal, Wiley-Eastern Limited 1999.

06. Organic Chemistry - I. L. Finar Vol.2, Longman, 1986.

07. Heterocyclic Chemistry - T.L. Gilchrist.

08. General Bio-chemistry - J. H. Weil, New Age International, 1997.

09. Aromatic Character - M. Badger, Cambridge University Press, 1966.

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PHYSICAL CHEMISTRY II – P13CH12

Semester : III **Core Course : X**

Code : P13CH12 **Credit: 5**

Instruction Hours/Week: 6

UNIT I: Group Theory

Elements of Group theory - Classes - group multiplication tables - properties of group, subgroup and isomorphism groups - symmetry elements and operations - point groups of molecules - Matrix representation of geometric transformation - Consequences of great orthogonality theorem and construction of character tables - bases for reducible and irreducible representations - direct product - Projection operators.Applications of Group theory to IR, Raman and Electronic spectra - SALC procedure -evaluation of energies and MO's for systems like ethylene, butadiene.

UNIT II: Quantum Chemistry-II

Application of SWE to simple harmonic oscillator (Hermite polynomial, eigen functions, eigen values) - rigid rotator with free axis (SWE in polar coordinates,separation of angular functions and their solutions, Legendre and associated Legendre polynomials, degeneracy of rotational states) - selection rules for rotational and vibrational transitions - Bohr's correspondence principle - hydrogen atom and hydrogen like systems, electron spin.Exactly solvable nature of systems - approximation methods - Many electron atoms -wave function - one electron orbital - Pauli principle and Slater determinant - Variation method - application to hydrogen and helium atom - pertubation method to non -degenarate systems.Hartree Fock Self consistent field methods - spin orbit interactions - L.S and J.J. coupling schemes - Vector model of the atom - term symbols

UNIT III: Molecular Spectroscopy-II

NMR: Spin and applied magnetic field - Larmor precession - Relaxation processes -PMR chemical shifts - spin spin interaction - FT NMR - multiple pulse NMR - ^{13}C NMR - Chemical exchange - evaluation of thermodynamic parameters in simple systems.

ESR: Basic principles - Zero field splitting and Kramer's degeneracy - Factors affecting the 'g' value - hyperfine splitting - spin Hamiltonian, spin densities and McConnell relationship, Measurement technique and applications.

UNIT IV: Electrochemistry-I

Ionics: Debye-Huckel theory - radius of ionic atmosphere and its calculation – Debye-Huckel-Onsager equation and its modifications - asymmetry and electrophoretic effects - Debye Falkenhagen and Wien's effects - Activity of ions in solutions - Debye Huckel limiting Law.Electrode - electrolyte equilibrium: Nernst equation derivation and its limitations - equilibrium electrode potentials - Calomel electrode, concentration cells - liquid junction potentials - Thermodynamic quantities from EMF data.Electrochemical energy - Storage system - Primary and secondary batteries –H_2-O_2 and Hydrocarbon-Oxygen fuel cells..

UNIT V: Statistical Mechanics

Statistical Mechanics: Basic concepts and classical statistics.Statistical Mechanics-calculation of thermodynamic probability of system- phase space-ergodic hypothesis-definition of micro and macro states- different methods of counting microstates- distinguishable and indistinguishable particles- classical statistics-derivation of Maxwell's Boltzmann distribution law-velocity and energy distribution.

Quantum Statistics: Bose-Einstein and Fermi-Dirac statistics- comparison of them with Boltzmann statistics- Application of BE statistics to photon gas and superfluidity of liquid helium-Application of FD statistics to electron gas and thermionic emission.

Reference:

01. F.A.Cotton, Chemical Applications of Group Theory, 2nd ed.,Wiley Eastern 1971.
02. A. K. Chandra, Introductory Quantum Chemistry, 4th ed., Tata McGraw Hill, 1994
03. D. A. Mcquarrie, Quantum Chemistry, University Science Books, 1983.
04. J. P. Lowe, Quantum Chemistry, Academic Press, 1978.
05. I. N. Levine, Quantum Chemistry, Allyn and Bacon, 1983.
06. P.W.Atkins, Physical Chemistry, ELBS and Oxford University Press,Oxford, 1983.
07. S. Glasstone, Introduction to Electrochemistry, Affiliated East-West Press, 1968.
08. D. R. Crow, Electrtochemistry

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PHYSICAL CHEMISTRY PRACTICAL I – P13CH13P

Semester : III & IV **Core Course: XI**

Instruction Hours/Week: 6 **Credit: 5**

Any ten experiments (to be decided by the course teacher) out of the following experiments.

a. Kinetics - Acid hydrolysis of ester- Comparison of strengths of acids.

b. Kinetics - acid hydrolysis of Ester- Determination of energy of activation (E_a).

c. Kinetics - Saponification of Ester- Determination of E_a by conductometry.

d. Kinetics - Persulphate- Iodine reaction- Determination of order, effect of ionic strength on rate constant.

e. Determination of molecular weight of substance by Transition Temperature method.

f. Determination of molecular weight of substances by Rast method.

g. Determination of Critical Solution Temperature (CST) of phenol-water system and effect of impurity on CST.

h. Study of phase diagram of two components forming a simple eutectic.

i. Study of phase diagram of two compounds forming a compound.

j. Study of phase diagram of three components system.

k. Determination of molecular weight of substances by cryoscopy.

l. Determination of integral and differential heat of solutions by colorimetry.

m. Polymerization- Rate of polymerization of acrylamide.

n. Distribution law- Study of association of benzoic acid in benzene.

o. Adsorption - Oxalic acid/Acetic acid on charcoal using freundlich isotherm.

References:

01. J. B. Yadav, " Advanced Practical Physical chemistry", 20th edn. GOEL publishing House, Krishna Pakashan Media Ltd., (2001).

02. Findlay's "Practical Physical Chemistry" Revised and edited by B. P. Levitt 9th ed., Longman, London, 1985.

03. J. N. Gurtur and R. Kapoor, "Advanced Experimental chemistry", Vol. I. Chand & Co., Ltd, New Delhi.

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PHYSICAL METHODS IN INORGANIC CHEMISTRY – P13CH14E

Semester : III **Elective Course: III**

Instruction Hours/Week: 6 **Credit: 4**

UNIT I: Electronic Spectroscopy

Microstates, terms and energy levels for d^1 - d^9 ions in cubic and square fields - intensity of bands - group theoretical approach to selection rules - effect of distortion and spin - orbit coupling on spectra - Evaluation of 10 Dq and β for octahedral complexes of cobalt

and nickel complexes - application to simple coordination compounds - Charge transfer spectra- electronic spectra of $[Ru(bpy)_3]^{2+}$.

UNIT II: Infrared and Raman Spectroscopy

Vibrations in simple molecules (H_2O, CO_2) and their symmetry rotation for molecular vibrations - group vibrations and their limitations - combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO_4^- - effect of coordination on ligand vibrations - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide - effect of isotopic substitution on the vibrational spectra of molecules - Vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment) - Applications of Raman Spectroscopy - Resonance Raman Spectroscopy.

UNIT III: NMR Spectroscopy

Examples for different spin systems - chemical shift and coupling constants (spin-spin coupling) involving different nuclei (^1H, ^{19}F, ^{31}P, ^{13}C) - interpretation and applications to inorganic compounds - effect of quadrupolar nuclei (^2H, ^{10}B, ^{11}B) on the ^1H NMR spectra, satellite spectra.Systems with chemical exchange - evaluation of thermodynamic parameters in simple systems - study of fluxional behaviour of molecules - an elementary treatment of second order spectra - examples - NMR of paramagnetic molecules - isotropic shifts - contact and pseudo contact interactions - Lanthanide shift reagents.

UNIT IV Electron Paramagnetic Resonance spectroscopy and magnetic properties

EPR spectroscopy: Theory of EPR spectroscopy - spin densities and McConell relationship - factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramer's degeneracy - spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II), and Cu(II) complexes - Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.Magnetic Properties: Types of magnetism-Dia-para-ferro and antiferrro magnetism. Magnetic properties of free ions - first order Zeeman effect - Second order Zeeman effect - states KT - states<<KT. Determination of Magnetic moments and their application to the elucidation of structures of inorganic compounds - temperature independent paramagnetism. Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds.

UNIT V: Mossbauer and NQR spectroscopy

Mossbauer spectroscopy - isomer shift - Doppler effect - magnetic interactions - Mossbauer emission spectroscopy - application to Iron and Tin compounds.NQR spectroscopy - characteristics of quadrupolar nucleus - effects of field gradient and magnetic field upon quadrupolar energy levels - NQR transitions - application to NQR spectroscopy.

References:

01. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd edn., Wiley Eastern company, London.

02. R. S. Drago, Physical Methods in Chemistry, W.B. Saunders Company, Philadelphia, USA.

03. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry" 5th Edition, Wiley-Interscience Publication, New York, 1990.

04. E. A. V. Ebsworth, Sructural methods in Inorganic chemistry, 3rd edn., ELBS Great Briton, 1987.

05. C. N. Banwell, Fundamentals of molecular spectroscopy, 3rd edn.., TMH, New Delhi, 1983.

06. Lewis and Wilkins, Modern Coordination Chemistry

07. P. J. Wheatley, "The Determination of Molecular Structure", Clarendon, Oxford, 1960.

08. G. M. Barrow, "Introduction to Molecular Spectroscopy," McGraw-Hill, NewYork, 1962.

09. A. E. Gillan and E. S. Stern, "Electronic Absorption Spectroscopy"' 2nd ed., Arnold, London.

10. K. Nakamoto, "Infraed Spectra of Inorganic and coordination compounds", Wiley, New York.

11. J. D. Roberts, "High Resolution Nuclear Magnatic Resonance", Mc Graw-Hill, New York.

12. T. P. Das and E. L. Hahn, "Nuclear Quadrupole Resonance Spectroscopy", Academic, New York.

13. H. E. Duckworth, "Mass Spectroscopy", Cambridge, New York.

14. B. N. Figgis and J. Lewis," The Magnetic properties of transitition metal complexes"' in Progress in Inorganic Chemistry", vol.6, ed. F. A.Cotton, Interscience, New York

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NANOMATERIALS AND SYNTHETIC ORGANIC CHEMISTRY – P13CH15E

Semester : III **Elective Course: IV**

Instruction Hours/Week: 6 **Credit: 4**

UNIT I: Nanomaterials - An Introduction and Synthetic Methods

Definition of nanodimensional materials - Historical milestones - unique properties due to nanosize, Quantum dots, Classification of nanomaterials. General methods of synthesis of nanomaterials:

Physical approaches- Chemical vapour deposition, Electro deposition and High-energy ball milling .Chemical approaches - Microwave irradiation, sol-gel, precipitation technology - Reverse micelle synthesis, Synthesis of Nanomaterials using microorganisms, Sonochemical synthesis.

Applications of nanomaterials: nanomaterials in medicine, in energy sector and in ceramics industries. Inorganic nanomaterials - typical examples - nano TiO2/ZnO. Organic nanomaterials - examples - Rotoxanes and Catenanes.

UNIT II: Techniques, Properties and Applications

Techniques for characterization of nanoscale materials. Principles of atomic force microscopy (AFM), Transmission Electron Microscopy (TEM) - Resolution and Scanning Transition Electron Microscopy (STEM), Scanning Tunneling Microscopy (STM), Scanning Near field Optical Microscopy (SNOM). Nanocapsules - cavitands - cucurbiturils, nanocatalysis.

UNIT III: Nanostructures

Carbon clusters: Discovery of C60 - alkali doped C60 - superconductivity in C60 - larger and smaller fullerenes.

Carbon nanotubes: Synthesis- single walled carbon nanotubes – structure and characterization - Mechanism of formation - chemically modified carbon nanotubes – doping - Functionalizing nanotubes - Application of carbon nanotubes.

Nanowires: Synthetic strategies - Gas phase and solution phase growth - Growth control - Properties.

UNIT IV: Disconnection Approach and Synthetic Strategies

Introduction to retrosynthetic analysis and disconnection approach - relay and convergent synthesis. Introduction to synthons, synthetic equivalents - target molecule - Umpolung - designing synthesis by disconnection approach.

Functional group interconversions - the importance of the order of events in organic synthesis - protecting group - principle, preparation and properties of alcohol, amine, carboxylic acids.

One group C-C disconnections in alcohols, olefins, ketones. Two group disconnections - 1,2 and 1,3 difunctional compounds. C-X disconnection - chemoselectivity (guidelines) - Robinson annulation.

UNIT V: Reagents for Reduction and Oxidation Reactions (with mechanism)

Reduction: Catalytic hydrogenation - Wilkinson catalyst - dehydrogenation, reduction with LAH, NaBH4, tertiary - butoxyaluminium hydride, $NaCNBH_3$, tributyltinhydride, hydrazines -wolff- kishner reduction, LDA, Gilman's reagent.

Oxidation: oxidation of hydrocarbons, Oxidation of alcohols- Chromic acid , oxidation of carbon-carbon double bond- $KMnO_4$, OsO_4, sharpless asymmetric epoxidation, Ozone, DDQ, dioxiranes, $Pb(OAc)_4$, SeO_2, ,peracids, Platinum - catalysed oxidation of alkenes.

References:

01. C. N. R. Rao, A. Muller, A. K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol. 1,2 Wiley- VCH, Weinheim, 2004.(Unit-I & Unit-III)

02. C. P. Poole, Jr., F. J. Owens, Introduction to Nanotechnology, Wiley Interscience, New Jersey, 2003. (Unit-I & Unit-III)

03. Principles of Nanoscience and Nanotechnology, M.A. Shah and Tokeer Ahamed (Unit-I)

04. Kenneth J. Klabunde (Ed), Nanoscale Materials in Chemistry, Wiley- Interscience, New York, 2001. (Unit-I)
05. T. Pradeep, Nano: The Essentials in Understanding Nanoscience and Nanotechnology, Tata McGraw Hill, New Delhi, 2007. (Unit-I & Unit-II)
06. H. Fujita (Ed), Micromachines as tools in nanotechnology, Springer-Verlag, Berlin, 2003.
07. Bengt Nolting, Methods in modern biophysics, Springer-Verlag, Berlin, First Indian Reprint, 2004. (Pages 102-146 for Unit II).
08. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties(Unit-II)
09. T. Tang and P. Sheng (Eds): Nano Science and Technology Novel Structures and Phenomena, Taylor & Francis, New York, 2004(Unit-II)
10. A. Nabok, Organic and Inorganic Nanostructures, Artech House, Boston, 2005. (Unit-I)
11. Nano letters - http://pubs.acs.org/journals/nalefd/index.html
12. Nanotation - http://www.acsnanotation.org/
14. Stuart Warren, Organic synthesis - the disconnection Approach, John Wiley & sons, 2004(Unit-IV)
15. Raymond K. Mackie & David M. Smith, Guidebook to Organic synthesis. (Unit- IV)
16. Jagdamba Singh and L. D. S. Yadav, Organic Syntheis, Pragati Prakashan, 2006. (Unit - IV)
17. W. Carouthers, Some modern methods of organic synthesis, Cambridge University Press, 1993. (Unit - IV & Unit - V)
18. H. O. House, Modern Synthetic Reactions, Allied Publishers, 1985. (Unit - V)
19. V. K. Ahluwalia and R. K. Parashar, Organic Reaction Mechanism, Narosa, 2002. (Unit -V)

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ORGANIC CHEMISTRY III – P13CH16

Semester : IV **Core Course: XII**

Instruction Hours/Week: 6 **Credit: 5**

UNIT I: Pericyclic Reactions and Optical Rotatory Dispersion and Circular Dichorism

Characteristics - classification - molecular orbital symmetry - frontier orbitals ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems - applications of frontier molecular orbital (FMO) and molecular orbital correlation diagram methods to eletrocyclic reactions (4n and 4n+2) system and cycloaddition reactions (2+2 and 4+2π electron system) - woodward hofmann rules - sigmatropic rearrangement (1,3 and 1,5 hydrogen shift) cope and claisen rearrangement (3,3 carbon shift) - chelotropic reactions.

Introduction to theory and terminology - circular birefringence - circular dichorism - cotton effect and ORD curves - comparison between ORD and CD and their inter relationship -

axial haloketone rule and octant rule - applications to determine the absolute configuration of monocyclic ketones and steroids.

UNIT II: Organic Photochemistry and Electron Spin Resonance Spectroscopy

Fundamental concepts - jablonski diagrams - photosensitization - photochemical reactions - photo reduction - photo oxidation, photo rearrangements - di- -methane rearrangement, photo reactions of ketones and enones - Norrish type I and II reactions - Paterno Buchi reaction - barton reactions - photochemistry of alkenes, dienes - photo addition reactions, photo chemistry aromatic compounds.Basic principles - comparison between ESR and NMR spectroscopy - hyperfine splitting - calculation of unpaired electron density on an atom in a delocalized system ($C_6H_6^-$, p-xylene anion, naphthalene radical ion) - structure of methyl radical, p-benzoquinone radical anion.

UNIT III: NMR Spectroscopy

^1H NMR spectroscopy - introduction - chemical shift, shielding, deshielding, chemical and magnetic non-equivalence of protons - spin-spin splitting - coupling constant - dependence of J on dihedral angle - vicinal and geminal coupling - karplus equation - factors influencing chemical shift - first and second order proton - simplification of complex. Spectra-double resonance techniques - contact shift reagents - chemical spin decoupling of exchangeable protons (OH, SH, COOH, NH, NH_2) - Nuclear Overhauser Effect 2D techniques (COSY, NOESY and ROSY).

C-13 NMR- Basic principles - FT - NMR relaxation - broad band decoupling - off resonance decoupling and calculation of chemical shift for simple aliphatic (olefin, alkynes, carbonyl carbon) and aromatic compounds - conformation and chemical shift correlation peak assignments. Importance of NOE phenomenon in ^{13}C spectroscopy.

UNIT IV: UV-Visible and Mass spectroscopy

Basic principles of electronic transitions - applications of UV-visible spectroscopy - woodward-fiescher scott rules - applications to conjugated dienes, trienes, polyenes - α-β-unsaturated carbonyl compounds. Conjugated cyclic ketones and acetophenones - aromatic hydrocarbons and heterocyclic systems - differentiation of position isomers and cis-trans isomers.Introduction - ion production - factors affecting fragmentation, ion analysis - ion abundance - base peak, isotopic peak, meta stable peak, parent peak - fragmentation of organic compounds with respect to their structure determination of common functional groups - molecular ion peak - McLafferty rearrangements. Nitrogen rule - high resolution mass spectroscopy.

UNIT V: Infrared Spectroscopy and Combined Spectroscopic Problems

Molecular vibrations - stretching vibrations - symmetric and asymmetric - bending vibrations - rocking, scissoring, wagging and twisting - finger print region - charactersitic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds - alcohols, ethers,

phenols and amines - detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, acids) - effect of hydrogen bonding (inter and intra molecular) and solvent effect on vibrational frequencies - overtones - fermi resonance.Calculation of double bond equivalents and its application in structural elucidation - problems involving combined UV, IR, NMR, CMR and mass spectra data.

References:

01. "Organic Photo Chemistry and Pericyclic reaction, M.G. Arora.

02. Organic Reactions and Orbital symmetry, T.L. Gilchrist and R.C. Storr. Cambridge, 1979.

03. The Conservation of Orbital symmetry, R.B. Woodward and R.Hoffmann, Academic Press, 1970.

04. Photochemistry and Pericyclic reactions. Jagdamba Singh and Jaya Singh - New Age International, 2005.

05. Organic Spectroscopy - Principles and Applications, Jag Mohan - Narosa, 2000.

06. Elementary Organic Spectroscopy (Principles and Chemical Application). Y. R. Sharma, S. Chand, 1992.

07. Organic Spectroscopy, William Kemp Macmillan, 1991.

08. Spectroscopy of Organic Compounds - P.S. Kalsi - New Age International, 2000.

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PHYSICAL CHEMISTRY PRACTICAL – II – P13CH17P

Semester : III & IV **Core Course: XIII**

Instruction Hours/Week: 6 **Credit: 5**

Any ten experiments (to be decided by the course teacher) out of the following experiments.

a. Conductometry - Acid- alkali titrations.

b. Conductometry - Precipitation tritrations.

c. Conductometry - Displacement titrations.

d. Conductometry - Determination of dissociation constant of weak acids.

e. Conductometry - Solubility product of sparingly soluble silver salts.

f. Conductometry- Verification of Onsager equation

g. Conductometry - Determination of degree of hydrolysis and hydrolysis constant of a substance.

h.Conductometry - To determine the relative strength of two acids.

i. Potentiometric titrations - Acid alkali titrations.

j. Potentiometric titrations - Precipitation titrations.

k. Potentiometric titrations - Redox titrations.

l. Potentiometry - Determination of dissociation constant of weak acids.

m. Potentiometry - Determination of solubility of silver salts.

n. Potentiometry - Determination of activity and activity coefficient of ions.

o. Potentiometry - pH titration of ortho -phosphoric acid.

p. Potentiometry- To determine the pH of a buffer solution using quinhydrone electrode.

References:

01. J. B. Yadav, " Advanced Practical Physical chemistry", 20th edn. GOEL publishing House, Krishna Pakashan Media Ltd., (2001).

02. Findlay's "Practical Physical Chemistry" Revised and edited by B. P. Levitt 9th ed., Longman, London, 1985.

03. J. N. Gurtur and R. Kapoor, "Advanced Experimental chemistry", Vol. I. Chand & Co., Ltd, New Delhi.

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PHYSICAL CHEMISTRY - III – P13CH18E

Semester : IV **Elective Course: V**

Instruction Hours/Week: 6 **Credit: 4**

UNIT I: Quantum Chemistry and Spectroscopy

MO and VB treatment of hydrogen molecule - HMO model for systems like ethylene and butadiene - concept of bond order and charge density - hybridization derivation of wave function for sp, sp^2 and sp^3 hybrid orbitals.

Photoelectron spectroscopy: basic principles - UPES, XPES and AES - valence and core binding analysis, Koopman's theorem - ESCA and Auger spectroscopy to the study of surfaces.

UNIT II: Statistical Thermodynamics

Partition functions: Translational, rotational, vibrational, electronic - calculation of enthalpy , internal energy, entropy and other thermodynamic functions - application of partition functions to mono and diatomic molecules.Heat capacity of solids: Einstein and Debye's treatments - concept of negative Kelvin temperature.Non-equilibrium thermodynamics: Thermodynamics of irreversible process - enthalpy production and entropy flow in open system - Onsager theory - phenomenological relations - Onsager reciprocal relations - steady state conditions.

UNIT III: Chemical Kinetics, Photochemistry and Radiation Chemistry

Fast reaction techniques: Flow methods: Stopped flow technique - Relaxation methods - Flash photolysis - Shock tube method - molecular beam method.

Photochemistry and Radiation chemistry: Photo physical process in electronically excited molecules - Jablonski diagram – Stern-Volmer equation - Chemical Actinometers - Lasers and their applications.

Radiation chemistry:- Sources of high energy radiation - radiolysis of water - solvated electrons - Scavenging techniques - Applications of radiation chemistry.

UNIT IV: Electrochemistry-II

Electro kinetic Phenomena: Theories of electrical double layer - Theory of multiple layers at electrode electrolyte interface - electro kinetic phenomena.

Processes at electrodes - the rate of charge transfer - current density – Butler-Volmer equation - Taft equation.

Electro chemical corrosion - construction and use of Pourbaix and Evans diagram - prevention of corrosion - electro chemical oxidation and reduction.

UNIT V: Electrochemistry-III

Principles and applications of Polarography - Instrumentation, Types of cells, advantages of dropping mercury electrode, interpretation of current voltage curves, determination of 'n' value, polarographic maxima. Cyclic voltammetry, advantages over polarography techniques - test of reversibility of electron transfer reactions.

References:

01. A. K. Chandra, Introductory Quantum Chemistry, 4th ed., Tata McGraw Hill, 1994

02. I. N. Levine, Quantum Chemistry, Allyn and Bacon, 1983

03. P. W. Atkins, Physical Chemistry, ELBS and Oxford University Press, Oxford,1983

04. J. Rajaram and J. C. Kuriacose, Thermodynamics for students of Chemistry - Classical, Statistical and Irreversible, Shobhan Lal Nagin, New Delhi, 1981

05. K. J. Laidler, Chemical Kinetics, 2nd ed, Tata McGraw Hill, 1975

06. A. A. Frost and R. G. Pearson, Kinetics and Mechanisms, John Willey & Sons, New York, 1953

07. K. K. Rohatgi and Mukerjee, Fundamentals of Photo Chemistry, Wiley Eastern Ltd (1986)

08. G. Hughes, Radiation Chemistry, Oxford University Press(1973)

09. S. Glasstone, Introduction to Electro Chemistry, Affiliated East-west Press,1968

10. D. R. Crow, Polarography of metal complexes, Academic Press, New York

11. Daniel C.Harris, Quantitative Chemical Analysis, 4th edn, W.H.Freeman and Company, New York,1995

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PROJECT WORK - P13CHP19

Semester : IV **Project**

Instruction Hours/Week: 12 **Credit: 5**

PROJECT WORK

(Dissertation 75 marks & Viva Voice – 25 Marks)

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