St. PETER'S UNIVERSITY

St. Peter's Institute of Higher Education and Research
(Declared under section 3 of UGC Act 1956)
Avadi, Chennai – 600 054.

M.Sc. (CHEMISTRY) PROGRAMME

(Full Time)

(I to IV SEMESTERS)

REGULATIONS AND SYLLABI

REGULATIONS – 2016

(Effective from the Academic Year 2016-'17)

M.Sc. CHEMISTRY

Regulations -2016

Regulations and Syllabi

(Effective from the Academic Year 2016-'17)

1. **Eligibility:** A Candidate who has passed B.Sc. Examination with Chemistry as main subject of study in the University or any of the B.Sc. Degree Examination with specialization such as Industrial Chemistry, Applied Chemistry, or any other specialization in Chemistry of other University recognized by this University as equivalent thereto, are eligible for admission to Two Year M.Sc. Programme in Chemistry.

2. **Duration**: Two years comprising 4 semester. Each semester has a minimum 90 working days with a minimum of 5 hours a day and a minimum of 450 hours per semester. Candidates who have completed the duration of the programme of study are permitted to appear for the arrear subjects examinations, if any within two years after the duration of the programme.

3. **Medium:** English is the medium of instruction and examination.

4. **Weightage for Continuous and End Assessment:** The weightage for Continuous assessment (CA) and End Assessment (EA) is 25: 75 unless the ratio is specifically mentioned in the scheme of Examinations. The Question Paper is to be set for a maximum of 100 Marks.

5. **Choice Based Credit System:** Choice Based Credit System is followed with one credit equivalent to one hour for a theory paper and two hours for a practical per week in a cycle of 18 weeks (that is, one credit is equal to 18 hours for each theory paper and one credit is equal to 36 hours for a practical in a semester) in the Time Table. The total credits for the programme (4 semesters) is 90.

6. **Scheme of Examinations**

I Semester

Code No.	Course Title		Credit	Marks		
Theory				**CA**	**EA**	**Total**
116CMPT01		Organic Chemistry-I	6	25	75	100
116CMPT02		Inorganic Chemistry-I	6	25	75	100
116CMPT03		Physical Chemistry-I	6	25	75	100
116CMPP01		organic Chemistry Practical I	2	25	75	100
116CMPP02		Inorganic Chemistry Practical I	2	25	75	100
		Total	**22**	**125**	**375**	**500**

II Semester

Code No.	Course Title		Credit	Marks		
Theory				**CA**	**EA**	**Total**
216CMPT01		Organic Chemistry-II	5	25	75	100
216CMPT02		Inorganic Chemistry-II	5	25	75	100
216CMPT03		Physical Chemistry-II	6	25	75	100
216CMPT04	Extra Disciplinary Activity - I: **Polymer Chemistry**		2	25	75	100
216CMPP01	Analytical Chemistry practical-I		2	25	75	100
216CMPP02	Physical Chemistry practical-I		2	25	75	100
		Total	**22**	**150**	**450**	**600**

Extra Disciplinary Activity - I

216CMPT04	**Polymer Chemistry**
216CMPT05	Chromatographic Techniques
216CMPT06	Analytical Techniques in Chemistry
216CMPT07	Environmental Chemistry

III Semester

Code No.	**Course Title**		**Credit**	**Marks**		
Theory				**CA**	**EA**	**Total**
316CMPT01		Organic Chemistry-III	5	25	75	100
316CMPT02		Inorganic Chemistry-III	5	25	75	100
316CMPT03		Physical Chemistry-III	6	25	75	100
316CMPT04	**Extra Disciplinary Activity - II:**		2	25	75	100
316CMPP01	Organic Chemistry Practical-II		2	25	75	100
316CMPP02	Inorganic Chemistry Practical-II		2	25	75	100
		Total	**22**	**150**	**450**	**600**

Extra Disciplinary Activity - II

316CMPT04	Materials Science
316CMPT05	Bioorganic Chemistry
316CMPT06	Research Methodology
316CMPT07	Bioinorganic Chemistry

IV Semester

Code No.	**Course Title**		**Credit**	**Marks**		
Theory				**CA**	**EA**	**Total**
416CMPT01		Organic Chemistry-IV	4	25	75	100
416CMPT02		Inorganic Chemistry-IV	4	25	75	100
416CMPT03		Physical Chemistry-IV	4	25	75	100
416CMPP01	**Practical**	Physical Chemistry practical-II	2	25	75	100
		Dissertation			65	
		Viva			10	
		Total	**24**	**125**	**375**	**500**

7. **Passing Requirements:** The minimum pass mark (raw score) be 50% in End Assessment (EA) and 50% in Continuous Assessment (CA) and End Assessment (EA) put together. No minimum mark (raw score) in Continuous Assessment (CA) be prescribed unless it is specifically mentioned in the Scheme of Examination.

8. **Grading System:** Grading System on a 10 Point Scale be followed with 1 mark = 0.1 Grade point to successful candidates as given below.

CONVERSION TABLE

(1 mark = 0.1 Grade Point on a 10 Point Scale)

Range of Marks	**Grade Point**	**Letter Grade**	**Classification**
90 to 100	9.0 to 10.0	O	First Class
80 to 89	8.0 to 8.9	A	First Class
70 to 79	7.0 to 7.9	B	First Class
60 to 69	6.0 to 6.9	C	First Class

50 to 59	5.0 to 5.9	D	Second Class
0 to 49	0 to 4.9	**F**	**Reappearance**

Procedure for Calculation

Cumulative Grade Point Average (CGPA)	=	$\frac{\text{Sum of Weighted Grade Points}}{\text{Total Credits}}$
	=	$\frac{\sum (CA+EA)\ C}{\sum C}$
Where Weighted Grade Points in each Course	=	Grade Points (CA+EA) multiplied by Credits
	=	(CA+EA)C
Weighted Cumulative Percentage of Marks(WCPM)	=	CGPAx10

C- Credit, CA-Continuous Assessment, EA- End Assessment

9. **Pattern of the Question Paper for Theory Subjects:** The question paper for End Assessment will be set for three hours and for the maximum of 100 marks with following divisions and details.

   Part A: 10 questions (with equal distribution to all units in the syllabus). Each question carries 2 marks.

   Part B: 5 questions with either or type (with equal distribution to all units in the syllabus). Each question carries 16 marks.

10. **Effective Period of Operation for the Arrear Candidates:** Two Year grace period is provided for the candidates to complete the arrear examination, if any.

Registrar

11.Syllabus

I Semester

116CMPT01 - ORGANIC CHEMISTRY - I

Objectives

This course aims to explain basic concepts in stereo chemistry and conformational analysis of organic molecules. In addition, the reaction mechanism and synthetic application of aliphatic and aromatic substitution reaction in organic synthesis will be discussed in detail.

Unit I: Stereochemistry

Introduction to optical activity and chirality, Stereomers-definition based on symmetry and energy criteria, Rotamers, prochiral carbons. Elements of chirality-Molecules with C, N, S based chiral centers. Configuration and conformational isomers. Absolute configuration-enatiomers- R, S nomenclature.

Steroisomerism due to molecular dissymmetry-allenes, biphenyls, spiro compounds, trans cyclooctene and cyclononene and molecules with helical structures enantiotopic, homotopic and diastereotopic hydrogens in compounds up to ten carbons only. Stereo specific and stereo selective reactions. Inter conversion of Sawhorse, Newman and Fischer projections. Molecules with more than one asymmetric center -definition of diasteroisomer-constitutionally symmetrical, unsymmetrical chiral compounds E.g. erythro and threo compounds.

Geometrical isomerism. E, Z nomenclature of olefins, geometrical and optical isomerism (if shown) of disubstituted cyclopropane, cyclobutane and cyclopentanes.

Unit II: Conformational analysis

Conformation of some simple, 1, 2-disubstituted ethane derivatives. Conformational analysis of disubstituted cyclohexanes and their stereo chemical features [cis, trans and optical isomerism (if shown) by these derivatives]. Conformation and reactivity of substituted cyclohexanols (oxidation and acylation), cyclohexanones and tert butyl cyclohexanols (reduction involving selectrides) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis). Conformation and stereochemistry of cis and trans decalin and 9-methyl decalin.

Unit III: Aliphatic Nucleophilic Substitution reactions

Kinetic Vs Thermodynamic control of product formation. Hammet equation. Derivation and free energy relationship, simple problems. Taft equation

S_N1, S_N2 and S_Ni mechanism - Nucleophile and leaving groups Stero chemistry and Ion pairs. Neighbouring group participation – by Aryl group, O, N, S halogens, single, double and triple bonds. Reactivity, structural, solvent and steric effects. Substituent effect on carbocations – cyclopropyl and carbonyl cations. Substitution in norbornyl system and at bridgehead carbon. Substitutions by ambident nucleophiles such as CN, NO_2, phenoxide and allkylation using dianion (EAA), acylation and alkylation of active methylene compounds.

Unit IV: Nucleophilic substitution reactions

Nucleophilic substitution at carbon which is doubly bonded to oxygen and nitrogen - alkylation and acylation of amines, halogen exchange, Von-Braun reaction. Enamines – synthesis-alkylation and acylation of enamines, hydrolysis of esters, Claisen and Dieckmann condensations.

Aromatic nucleophilic substitution - methods of generation of benzyne intermediate and reactions of aryne intermediates. Nucleophilic substitution involving diazonium ions. Aromatic nucleophilic substitution of activated halides. Ziegler alkylation. Chichibabin reaction.

Unit V: Aromatic electrophilic substitution reactions

The arenium ion mechanism. Orientation and reactivity (ortho, meta and para directing groups). . Typical reactions to be studied - nitration, halogenation, alkylation, acylation and diazonium coupling. Formylation reactions - Gatterman, Gatterman-Koch, Vilsmeyer-Hack & Reimer-Tieman Reaction. Synthesis of di & tri substituted benzenes (symmetrical tribromobenzene, 2-amino-5-methylphenol, 3-nitro-4-bromobenzoicacid, 3, 4-dibromonitrobenzene, 1, 2, 3 - trimethylbenzene) starting from benzene or any mono substituted benzene. Electrophilic substitution of furan, pyrrole, thiophene, pyridine and pyridine-N-oxide.

Text Books:-

1. E. Eliel, S.H.Wilen and L.N.Mander, 1994, Stereochemistry of Carbon Compounds, 2nd Edition, John Wiley & Sons, New York
2. D.Nasipuri, 1994, Stereochemistry of Organic Compounds, 2nd Edition,Wiley Eastern Ltd, New Delhi
3. PS. Kalsi, 1993, Stereochemistry, Conformation Analysis and Mechanism, 2nd Edition, Wiley Eastern Limited, Chennai
4. P.S. Kalsi, 1994, Stereochemistry and Mechanism Through Solved Problems Wiley Eastern Ltd.
5. Niel Isaacs, 1987, Physical Organic Chemistry, ELBS Publications
6. R.Bruckner, 2002, Advanced Organic Chemistry, Reaction Mechanism, Elsevier, New Delhi
7. F.A. Carey and R.J. Sundberg, 2001, Advanced Organic Chemistry, Part A and Part-B, 4th Edition, Plenum Press, New York
8. J. March, 1992, Advanced Organic Chemistry, 4th Edition, John Wiley& Sons, Singapore.
9. T.L. Gilchrist and C.W. Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London.
10. T.L. Gilchrist, 1992, Heterocyclic Chemistry, 2nd Edition, Longman, Essex, England
11. 11. J.A.Joule and K.Mills, 2000, Heterocyclic Chemistry, 4th Edn, Backwell Science Publishers, England.

Websites:-

1. http :// info dome . sdsu, ./research/ guides/ science/ org chemistryblr. html
2. http :// www.liv.ac.uk/chemistry/links /reactions.html
3. http ://orgchem.chem..uconn.edu/namereact/named.html
4. www.gcocities.com/ chempen softwar4ee/reactions.html

116CMPT02 - INORGANIC CHEMISTRY - I

Objectives

To impart the theories about bonding and structure of various inorganic compounds and few analytical techniques. The basics of reaction Mechanisms in coordination chemistry are also introduced.

Unit I: Bonding in Inorganic compounds

Poly acids: Isopolyacids and heteropolyacids of vanadium, chromium, molybdenum and tungsten.
Inorganic Polymers: Silicates, structure - properties - correlation and applications - molecular sieves, polysulphur - nitrogen compounds and poly - organophosphazenes.

Unit II: Boron compounds and clusters

Boron hydrides: Polyhedral boranes, hydroborate ions, carboranes and metallo carboranes. Wade's rules, preparation and reactions of Boron hydrides.

Metal Clusters: Chemistry of low molecularity metal clusters upto trinuclear metal clusters; multiple metal-metal bonds.

Unit III: Nano Material chemistry

Synthesis and Properties - Metallic nanoparticles – gold and silver – Nanorods and Nanotubes – Nanostructures – One, two and three dimensional – semiconductor quantum dots – carbon nanotubes, graphene – Core-shell and Quantum well structures.

Unit IV: Theories of coordination

Inadequacies of VB Theory- Crystal field theory- d-orbital splitting; octahedral, tetrahedral and square planar-LFSE, spectro chemical series-- Applications of crystal field theory – Spectral properties, magnetic properties-low spin and high spin complexes, thermodynamic properties and structural aspects: Ligand Field Theory**.** MO theory – LCAO method – Sigma and pi-bonded complexes.

Unit V: Stability and stereo isomerism of coordination complexes

Stability of complexes: thermodynamic stability – stepwise and overall stability constants, their relationships, factors affecting the stability, HSAB approach , chelate effect, importance of chelates.
Macrocyclic ligands; types; schiff bases; crown ethers; cryptands;
Chelating agents; types of EDTA titrations; direct and back titrations; replacement titrations; masking and demasking reagents.
Determination of stability constants by spectrophotometric, polarographic and potentiometric methods.
Stereochemical aspects; Stereoisomerism in inorganic complexes; isomerism arising
out of ligand and ligand conformation; chirality and nomenclature of chiral complexes; optical rotatory dispersion and circular dichroism.

Text Books:-

1. J.E. Huheey, 1993, Inorganic Chemistry - Principles, Structure and
2. Reactivity; IV Edition, Harper Collins, NY.
3. F.A. Cotton and G. Wilkinson, 1988, Advanced Inorganic Chemistry - A
4. Comprehensive Text, V. Edition, John Wiley & Sons.
5. K.F. Purcell and J.C. Kot, 1977, Inorganic Chemistry - WB Saunders Co.,

6. USA.
7. M.C. Day and J. Selbin, 1974, Theoretical Inorganic Chemistry, Van
8. Nostrand Co., NY.
9. G.S. Manku, 1984, Inorganic Chemistry, TMG Co.,
10. D.A. Skoog, 1985, Principles of Instrumental methods of Analysis, III
11. Edition, Saunders College Publication.
12. Willard Merrit, Dean and Settle, 1986, Instrumental methods of Analysis, VI Edition CBS Publication.
13. A.I. Vogel, 1985, 1976, Text Book of Qualitative Inorganic Analysis, ELBS III Edition, and IV Edition.
14. D.A. Skoog D.M. West, 1982, Fundamental of Analytical Chemistry, IV Edition, Holt Reinheart & Winston Publication.

Suggested Reference Books:-

1. D.F. Shrivers, P.W. Atkins and C.H. Langfor 1990, Inorganic Chemistry, CH Langford, OUP
2. N.N. Greenwood and Earnshaw, 1984, Chemistry of the Elements, Pergamon Press, NY.
3. F.A. Kettle, 1973, Coordination Chemistry, ELBS.
4. K. Burger, 1973, Coordination Chemistry, Burtterworthy.
5. Basolo and R.G. Pearson, 1967, Mechanism of Inorganic Reactions, Wiley,
6. NewYork.
7. R.Sarker, general and Inorganic chemistry, (Parts I and II), New Book Agency,
8. Calcutta
9. G.D. Christian & J.E.O. Reily, 1986, Instrumental Analysis, II Edition, Allegn
10. Becon.
11. H.A. Strobel, 1976, Chemical Instrumentation, Addison - Wesley Publ. Co. Kolthoff and Elwing (all series), Treatise on Analytical Chemistry.
12. Wilson and Wilson series, Comprehensive Analytical Chemistry.
13. R.C. Kapoor and B.S. Aggarwal, Ms. 1991, Principles of Polarography, Wiley Eastern Limited.

116CMPT03 - PHYSICAL CHEMISTRY - I

Objectives
To learn the basic concepts in chemical kinetics and group theory and the inadequacy of classical mechanics leading to the formation of quantum mechanics. Mathematical basic for quantum mechanics must be taught.

Unit I: Chemical Kinetics - I
Effect of temperature on reaction rates - collision theory - molecular beams - collision cross sections - effectiveness of collisions - probability factors - potential energy surfaces – transition state theory - partition functions and activated complex. Eyring equation - estimation of free energy, enthalpy and entropy of activation and their significance.

Unit II: Chemical Kinetics - II
Reactions in solutions - effect of pressure, dielectric constant, ionic strength and salt effect - kinetic isotopic effects - linear free energy relationships-Hammett and Taft equations - Homogeneous catalysis - Acid base catalysis - mechanisms and Bronsted catalysis law.

Unit III: Group theory - I
Symmetry elements and operations. Concepts of groups, Sub groups, class, order, Abelian and Non-Abelian point groups. Products of symmetry operations and group multiplication table, point groups-identification and determination-reducible and irreducible representations-Direct product representation-orthogonality theorem and its consequences-character table – construction(NH_3, H_2O). Symmetry adapted linear combinations of atomic orbitals (water as example)

Unit IV: Group theory - II
Hybrid orbital in non-linear molecules (CH_4, XeF_4, BF_3, SF_6 and NH_3). Determination of representations of vibrational modes in non-linear molecules (H_2O, CH_4, XeF_4, BF_3, SF_6 and NH_3)
Symmetry selection rules for infrared, Raman and electronic Spectra - mutual exclusion principle. Electronic Spectra of Ethylene and formaldehyde-Applications of group theory.

Unit V: Quantum Chemistry - I
Inadequacy of classical theory - black body radiation, photo electric effect - the Compton effect - Bohr's Quantum theory and subsequent developments -wave particle duality- de Broglie equation, Heisenberg uncertainty principle.

Text Books:-

1. G.K. Vemulapalli, 2000, Physical Chimistry, Prentice - Hall.
2. J. Rajaram and J.C. Kuriacose, 1993, Kinetics and mechanism of chemical transformations, MacMillan India Ltd.
3. K.J. Laidler, 1987, Chemical Kinetics, Harper and Row, New York.
4. K. L. Kapoor, 2001, A Text book of Physical Chemistry, Macmillan India
5. Ltd.
6. V. Ramakrishnan and M.S. Gopinathan, 1988, Group Theory in Chemistry,
7. Vishal Publications.
8. P.W. Atkins, 1990, Physical Chemistry, Oxford.

9. K.V. Raman, 1990, Group theory and its applications to Chemistry, Tata
a. McGraw Hill.
10. 8. D.A. McQuarrie, 1983, Quantum Chemistry, University Science Books, Mil
a. Valley, California.
11. I.N. Levine, 1983, Quantum Chemistry, Allyn and Bacon, Boston.
12. R. Anantharaman, 2001, Fundamentals of quantum chemistry, Macmillan India
13. Limited.
14. R.K. Prasad, 1992, Quantum Chemistry, New Age, India.

Suggested Reference Books:-

1. W.J. Moore, 1972, Physical Chemistry, Orient Longman, London.
2. L.K. Nash, 1962, Elements of Chemical Thermodynamics, Addision Wesley.
3. G.M. Barrow, 1988, Physical Chemistry, McGraw Hill.
R.G. Frost and Pearson, 1981, Kinetics and Mechanism, Wiley, New York.
4. Moore and R.G. Pearson, 1981, Kinetics and Mechanism.
5. I. Amdur and G.G. Hammes, 1968, Chemical Kinetics, Principles and selected
6. topics, McGraw Hill, New York.
7. G.M. Harrus, 1966, Chemical Kinetics, D.C. Health and Co.
8. F.A. Cotton, 1971, Chemical Application of Group Theory, John Wiley and Sons
9. Inc., NewYork.
10. Alan Vincent, 1977, Molecular symmetry and Group theory-programmed
11. introduction to Chemical Aplications, Wiley, New York.

PRACTICAL

116CMPP01 - ORGANIC CHEMISTRY PRACTICAL I

Objectives

To train the students to synthesize an organic compound in single step and to carry out the qualitative analysis of binary organic mixture.

I. Analysis of the organic mixture

1. Separation and Identification of components in a two component mixture and preparation of their derivatives.
2. Determination of b.p./ m.p. for purified components and m.p. of the derivatives.

II. Synthesis of organic compounds involving single step (Any Six)

1. Preparation of o-benzylbenzoic acid
2. p-Nitrobenzoic acid from p-Nitrotoluene
3. Anthroquinone from anthracene
4. Benzhydrol from benzophenone
5. m-Nitroaniline from m-dinitrobenzene
6. 1, 2, 3, 4-Tetrahydrocarbozole from cyclohexanone
7. p-chlorotoluene from p-toluidine
8. 2, 3-Dimethylindole from phenyl hydrazine and 2-butanone (boiling acetic acid)
9. Methyl orange from sulphanilic acid
10. Diphenyl methane from benzyl chloride

Recommended Books

1. Arthur I. Vogel, A Text Book of Practical Organic Chemistry.
2. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern Limited.
3. Mann and Saunders, Laboratory manual of Organic Chemistry

116CMPP02 - INORGANIC CHEMISTRY PRACTICAL I

Objectives:
To train the candidate in preparing inorganic compounds, the detection and identification of **4** cations by semi micro method.

Unit I:-
Semi micro qualitative analysis of mixtures containing two common and two rare cations. The following rare cation are included: W, Mo, Ti, Te, Se, Ce, Th, Zr, V, U and Li.

Unit II: Preparation of the following:-

1. Tris (thiourea) copper (I) chloride
2. Potassium tris (oxalato) chromate (III) trihydrate
3. Tris (thiourea) copper (I) sulphate
4. Potassium tris (oxalato) aluminate (III) trihydrate.

Text Books:-

1. Vogel, Text book of Inorganic quantitative analysis.
2. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.

Semester II

216CMPT01 - ORGANIC CHEMISTRY - II

Objectives

This paper explains the basic concepts of addition reaction of carbon carbon double bond and elimination reactions. In addition mechanism of some of the important rearrangements in organic chemistry will be discussed. The salient features of oxidation and reduction reactions in organic synthesis are discussed at the end.

Unit I: Addition to carbon-carbon and carbon-hetero multiple bonds: I

Nucleophilic addition to carbonyls and Stereo Chemical aspects through various model (Cram/Cram chelation/Felkin – Anh model)-Crams rule- Prevost rule-Re face-si face on addition reaction.
Mechanism of electrophilic, nucleophilic and neighbouring group participation in addition reactions. Addition of halogen and nitrosyl chloride to olefins, hydration of olefins and acetylenes, hydroboration, Lithium and boron enolates in aldol, Michael reactions. Alkylation and acylation using Lithium enolates, hydrogenation of ethylene and acetylene- partial reductions- Homogeneous hydrogenation- Wilkinson's catalyst.

Unit II: Addition to carbon-carbon and carbon-hetero multiple bonds: II

Ylides: Chemistry of phosphorous and sulfur ylides – Wittig and related reaction, Peterson Olification.

Diels Alder reaction, 1, 3-dipolar additions, carbenes and carbenoids - addition to double bonds - Simmon Smith reaction, Mannich, Knoevengal, Stobbe condensation, Shapiro reaction, Julia olefination, Acyloin condensations, Darzen, and benzoin reactions. Stereochemical aspects to be studied wherever applicable - Nitrenes : Methods for generating carbenes and nitrenes and their reactions.

Unit III: Elimination and Free radical reactions

E1, E2 and E1cB mechanism - Orientation of the double bond. Regio selectivity and stereoselectivity of elimination reactions in cyclic systems, pyrolytic eliminations. Chugaev, Hofmann and Cope Elimination.
Long and short lived free radicals - methods of generation. Adddition of free radicals to olefinic double bonds. Sandmayer - Gombereg-Gauchmann, Pschorr, Ulmann and Hunsdicker reactions.

Unit IV: Molecular rearrangements

A detailed study of the mechanism of the following rearrangements with suitable examples Pinacol-Pinacolone (examples other than tetramethyl ethylene glycol) - Wagner-Meerwein, Demjanov, dienone-phenol, Favorski, Baeyer-Villiger, Cope, Claisen, Stevens, Sommelet-Hauser (in cyclic systems also) and Von Richter rearrangements.

Unit V: Oxidation and reduction reactions

Oxidation: Mechanism - study of the following oxidation reactions - oxidation with LTA, SeO_2, DDQ, Oxalyl chloride, Dess-martin reagent DMSO in combination with DCC or acetic anhydride in oxidizing alcohols – Hydroxylations with – OsO_4, $KMnO_4$, Woodward prevost, epoxidation (per oxides/per acids). Sharpless epoxidation.

Reductions: Synthetic importance of Clemensen and Wolf-Kishner reductions and its Modifications, Birch reduction, MPV reduction.

Text Books:-

1. R.Bruckner, 2002, Advanced Organic Chemistry, Reaction Mechanism, Elsevier, New Delhi
2. F. A . Carey and R.J. Sundberg, 2001, Advanced Organic Chemistry, Part A and Part-B, 4th Edition, Plenum Press., New York
3. J.March, 2002, Advanced Organic Chemistry, 4th Edition, John Wiley & Sons Singapore.
4. T.L. Gilchrist and C.W. Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London.
5. Niel Issacs, 1987, Physical Organic Chemistry, ELBS Publications.
6. W. Carruthers, 1993, Some Modern Methods of Organic Synthesis, 3rd Edition, Cambridge University Press.
7. Reduction:- Hydride transfer reagents.
8. $NaBH_4$, $LiAlH_4$, DIBAL-H, Red-Al, Selectrides, Et_3SiH and Bu_3SnH
9. H.O. House, 1972, Modern Synthetic Reactions, The Benjamin Cummings Publishing Company, London.

Websites:-

1. http :// info dome . sdsu, ./research/ guides/ science/ org chemistryblr. html
2. http :// www.liv.ac.uk/chemistry/links /reactions.html
3. http ://orgchem.chem..uconn.edu/namereact/named.html
4. www.gcocities.com/ chempen softwar4ee/reactions.html

216CMPT02 - INORGANIC CHEMISTRY - II

Objectives
The student can gain the knowledge and understanding of all aspects of inorganic polymers, solid state and nuclear chemistry.

Unit I: Coordination chemistry – Reaction mechanisms
Electron transfer reactions; outer and inner sphere processes; atoms transfer reaction, complementary and non-complementary reactions.
Formation and rearrangement of precursor complexes, binding ligand, successor complexes, Marcus theory.

Unit II: Substitution reactions in coordination compounds
Substitution Reactions : Substitution in square planar complexes, reactivity of platinum complexes, influence of entering, leaving and other groups, trans-effect, substitution of octahedral complexes of cobalt and chromium, replacement of coordinated water, solvolytic (acids and bases) reactions applications in synthesis (platinum and cobalt complexes only).
Rearrangement in 4 and 6 coordinate complexes: reaction at coordinated ligands-template effect.

Unit III: Solid State Chemistry
Preparation Methods: Ceramic method – Sol-gel method – Hydrothermal synthesis –chemical vapour deposition: Structure of Solids: Structure of ZnS, Rutile, Pervoskite, Cadmium iodide and nickel arsenide; spinels and inverse spinels; defects in solids, non-stoichometric compounds - High Temperature Superconductors
Band theory, Semiconductors, Superconductors, Solid State Electrolytes, Types of Magnetic Behaviour - Dia, Para, Ferro, Antiferro and Ferrimagnetism, Hysterisis, Solid State Lasers, Inorganic Phosphorus, Ferrites, Garnets.
Reactions in solid state and phase transitions, diffusion, diffusion coefficient, diffusion mechanisms, vacancy and interstitial diffusion, formation of spinels.
Solid solutions: Order-disorder transformations and super structure.

Unit IV: Nuclear Chemistry
Nuclear properties-nuclear spin and moments, origin of nuclear forces, salient features of liquid drop and shell models.
Types of radioactive decay: Orbital electron capture, nuclear isomerism, internal conversion, detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M., Scintillation and Cherenkov counters; Accelerators- Linear and Cyclotron
Nuclear reaction: Types, reaction cross section, Q-value, threshold energy, compound nucleus theory: high nuclear reactions, nuclear fission and fusion reactions as energy sources; photonuclear and thermo nuclear reactions. Components of nuclear reactors – the fast breeder reactor – nuclear reactors in India.

Unit V: Nuclear Chemistry Application
Radioactive tracers: Preparations - principles of tracer technique - application of tracers in the study of reaction mechanism and in analytical chemistry - neutron activation analysis, isotope dilution analysis - radio chemical determination of age of geological specimen. Tracers as applied to industry and agriculture - radioactive tracer in the diagnosis and treatment in the field of medicine.

Text Books:-

1. K.F. Purcell and J.C. Kotz, 1977, Inorganic Chemistry WB Saunders Co., U.S.A.
2. J.E. Huheey, 1993, Inorganic Chemistry, IV Edition, Harper and Collins, NY.
3. F.A. Cotton and G.W. Wilkinson, 1988, Advanced Inorganic Chemistry - A Comprehensive Text; John Wiley & Sons.
4. B.E. Dogulas DH MX Daniels and Alexander, 1983, Concepts and Models of Inorganic Chemistry, Oxford IBH.
5. W.U. Mallik, G.D. Tul, R.D. Madan, 1992, selected topics in Inorganic Chemistry, S. Chand & Co., New Delhi.
6. A.R. West, 1991, Basic Solid State Chemistry, John Wiley.
7. W.E. Addison, 1961, Structural Principles in Inorganic Chemistry, Longman.
8. M. Adams, 1974, Inorganic Solids, John Wiley Sons.
9. S. Glasstone, Source Book on Atomic Energy, East West Press.
10. C.R. Choppin and J. Ryd Berg: Nuclear Chemistry - Theory and
    i. Applications, Pergamon Press.
11. B.G. Harvey, Introduction to Nuclear Physics and Chemistry Prentice Hall, 1962.

Suggested Reference Books:-

1. S.F.A. Kettle, 1973, Coordination Chemistry, ELBS.
2. B.N. Figgis, 1966, Introduction to Ligand Fields, Interscience.
3. M.N. Hughes, 1982, The Inorganic Chemistry of Biological processes, II Edition, Wiley London
4. D. Nicholas, 1974, Complexes of First Row Transition Elements.
5. M.C. Shrivers, PW. Atkins, CH Langford, 1990, Inorganic Chemistry, OUR
6. M.C. Day and J. Selbin, 1974, Theoretical Inroganic Chemistry, Van Nostrand Co., NY.
7. G.S. Manku, 1984, Inorganic Chemistry, TMH.
8. U. Sathyanarayana - Essentials of Biochemistry, Books and Allied (P) Ltd.
9. A.F. Wells, - 1984, Structural Inorganic Chemistry, V. Edition, Oxford
10. A.R. West, 1990, Solid State Chemistry, John Wiley.
1. G.D.Christian & J.E.O. Reily, 1986, Instrumental Analysis, II Edition, Allegn Recon.
2. H.A. Strobel, 1976, Chemical Instrumentation, Addition- Wesely Publ. Co.
3. Kolthoff and Elwing (All Series) - Treatise on Analytical Chemistry.
4. Willson Series - Comprehensive Analytical Chemistry.
5. H.A.O. Hill and P. Day, 1968, Physical methods in Advanced Inorganic Chemistry, JohnWiley.
6. K. Burger, 1973, Coordination Chemistry, Experimental methods, Butterworths.
7. C.N.R. Rao, J.R. Ferraro, 1970, Spectroscopy in Inorganic Chemistry, Vol. I and Vol. II, Academic Press.
8. G. Aruldas, Molecular Structure and Spectroscopy, Prentice Hall.
9. E.L. Mutterties, 1975, Polyhedral Borneds, Academic Press, NY.
10. NH Ray, 1978, Inorganic Polymers, Academic Press.

216CMPT03 - PHYSICAL CHEMISTRY - II

Objectives

To learn the concepts in enzyme kinetics, surface reactions and fast reactions, and also to understand the formulation and applications of quantum mechanics in atomic and molecular structure. In addition to learn fundamentals of spectroscopy.

Unit I: Chemical Kinetics - III

Catalysis by Enzymes-rate of enzyme catalyzed reactions, Michaelis-Menten equation effect of substrate concentration, pH and temperature - inhibitions of enzyme catalyzed reactions – three types with mechanism.

Heterogeneous catalysis, Langmuir and BET adsorption isotherms- Kinetics of Heterogeneous catalysis, Unimolecular and Bimolecular reaction. Langmuir-Rideal and Langmuir-Hinshelwood mechanisms. Adsorption coefficient and its significance. Kinetics and mechanism of surface reactions-catalysis by metals, Hydrogenations and semiconductor oxides.

Unit II: Chemical Kinetics - IV

Kinetics of complex reactions – reversible, consecutive and parallel reactions. Chain reactions: general treatment. Rice Herzfeld Mechanism - Decomposition of acetaldehyde and hydrobrominations. Comparison of HCl and HBr formation and explosion limits.

Study of fast reactions-relaxation methods-temperature and pressure jump -stopped flow and flash photolysis methods.

Unit III: Quantum Chemistry - II

Quantum mechanical postulates- Eigen value and function - the Schrodinger wave equation-elementary applications of Schrodinger's equation-the particle in a box (one, two and three dimensional cases) - particle in a ring.

Unit IV: Quantum Chemistry - III

The harmonic oscillator- the rigid rotor- the hydrogen atom- the Schrodinger equation for hydrogen atom- angular momentum - term symbols -the solution- the origin of quantum numbers (angular momentum and spin) -their physical significance.

Unit V: Spectroscopy I

Electromagnetic radiation: Quantization of energy- rotational, vibrational and electronic energy levels and transitions in molecules- regions and representation of spectra. Resolution and intensity of spectral transition: signal to noise ratio- width of spectral lines- collision broadening – Doppler broadening – Heisenberg uncertainty principle – intensity of spectral lines- selection rules and transition probability- transition moment integral- Eienstein absorption coefficient.

Electronic spectra of polyatomic molecules, Franck-condon principle- selection rules – types of transition in saturated and unsaturated hydrocarbons, effect of conjugation and solvent effects.

Text Books:-

1. J.Rajaram and J.C.Kuriakose, 1993, Kinetics and mechanism of chemical transformations, Macmillan India Ltd.
2. K.J.Laidler, 1987, Chemical Kinetics, Harper and Row, New York.
3. D.A. McQuarrie, 1983, Quantum Chemistry, University Science Books, Mil Valley, California.
4. I.N. Levine, 1983, Quantum Chemistry, Allyn and Bacon, Boston.
5. R. Anantharaman, 2001, Fundamentals of quantum chemistry, Macmillan India Limited.
6. R.K. Prasad, 1992, Quantum Chemistry, Wiley Eastern, New Delhi.

Suggested Reference Books:-

1. R.G.Frost and Pearson, 1961, Kinetics and Mechanism, Wiley, New York.
2. W.J.Moore and R.G.Pearson 1981, Kinetics and Mechanism.
3. R.K.Prasad, 1992, Quantum Chemistry, Wiley Eastern, New Delhi.
4. J.Goodman, 1997, Contemporary Quantum Chemistry, An Introduction, Plenum Press, New York.
5. R.Mcweeny, 1979, Coulon's Valence, ELBS Oxford University Press.
6. F.J.Bockhoff, 1976, Elements of Quantum theory, Addison Wesley, Reading Mass.
7. P.W.Atkins, 1990, Physical Chemistry, Oxford University Press.
8. H.Eyring, J.Walter and G. Gimball, 1944, Quantum Chemistry, John Wiley and Sons, New York.
9. L.S.Pauling and F.B.Wilson, 1935, Introduction to Quantum mechanics, Mc Graw Hill Book Company, New York.
10. P.W.Atkins, 1983, Molecular Quantum Mechanics, Oxford University Press, Oxford.

EXTRA DISCIPLINARY ACTIVITY – I

216CMPT04

CHROMATOGRAPHIC TECHNIQUES

Objectives
This paper enables a student to understand the basic principles of various chromatographic techniques and also instrumentation.

Unit I: Chromatography – General
Chromatographic methods, general aspects of chromatography, Types and mechanism.

Unit II: Column Chromatography (CC)
Column chromatography: construction and operation of column, choice of adsorbents and applications. Ion exchange chromatography: Anion & cation exchangers techniques and applications.

Unit III: Paper Chromatography (PC)
Paper chromatography: Principles, method, recent advancements and applications. Thin layer chromatography: Techniques, choice of adsorbents and applications.

Unit IV: Gas-liquid Chromatography (GLC)
Gas-liquid Chromatography: Principles, Retention Volumes, Instrumentation, Carrier Gas, Columns, Stationary Phase, Detectors, Thermal Conductivity, Flame Ionization, Electron Capture and applications.

Unit V: High Performance Liquid Chromatography (HPLC)
High Performance Liquid chromatography: scope, column efficiency, instrumentation, pumping systems, column packing, detectors and applications.

Text Books:-

1. Vogel's, 2000, Text book of Quatitative Chemical Analysis, Sixth Edition, Pearson Education Limited, London.
2. D. A. Skoog and J. J.Leary, 1971, Principles of Instrumental Analysis, Fourth Edition, Saunders College Publishing, US.

ANALYTICAL TECHNIQUES IN CHEMISTRY

Objectives

The course aims to explain various analytical techniques useful for chemistry. Colorimetric analysis and spectral techniques such as UV-Vis, IR, NMR, NQR, EST, TGA, MS, X-ray and Photoelectrons spectroscopy are objective of students learning.

Unit I: Colorimetric analysis, UV-Vis, IR and Raman spectrum

Colorimetric analysis and UV-Visible spectroscopy: Beer Lambert's law, Principles of single and double beam instruments – applications for analysis of inorganic and organic samples.
Infrared spectrophotometric analysis – principle, instrumentation and structure determination.
Raman Spectra – principle, basic instrumentation and structural analysis.

Unit II: NMR and NQR

Nuclear Magnetic Resonance – Principle, instrumentation, structure determination. NMR of ^{1}H, ^{13}C, ^{31}P, ^{19}F.
NQR - Nitrosyl compounds, Mossbauer of Fe and Sn systems.

Unit III: ESR and Magnetic properties

Electron Spin Resonance – Principle, instrumentation, applications to coordination compounds.
Magnetic Susceptibility and measurements- Guoy method, Faraday method-applications.

Unit IV: TGA, DTA and Mass Analysis

Thermo gravimetric and differential thermal analysis, thermometric titrations, differential scanning colorimetry – basic instrumentation and applications.
Mass Spectrometry- Principle, basic instrumentation, fragmentation patterns -structural determination of organic molecules.

Unit V: Atomic absorption spectroscopy and Photoelectron spectroscopy

Atomic absorption spectroscopy: Theory, atomizers, flame and electro thermal. radiation sources, instrumentation, spectral and chemical interferences and application.
Photoelectron spectroscopy (UV and X-Ray)-photo electron spectra-Koopman's theorem, fine structure in PES, chemical shift and correlation with electronic charges.

Text Books:-

1. D.A .Skoog, 1985, Principles of Instrumental Methods of analysis, III Edition, Saunders College Publ.
2. Willard Merrit, Dean and Settle, 1986, Instrumental methods of analysis, VI Edition, CBS Publ.
3. A.I. Vogel, 1976, Textbook of Qualitative Inorganic Analysis, III Edition, ELBS.
4. D.A. Skoog and D.M. West, 1982, Fundamentals of Analytical Chemistry, IV
5. Edition, old Reinhord & Winston, Publication.

Suggested Reference Books:-

1. G.D.Christian & J.E.O. Reily, 1986, Instrumental Analysis, II Edition,
2. Allegn Recon.
3. H.A. Strobel, 1976, Chemical Instrumentation, Addition- Wesely Publ Co.

4. Kolthoff and Elwing (All Series) - Treatise on Analytical Chemistry.
5. Willson Series - Comprehensive Analytical Chemistry.
6. H.A.O. Hill and P. Day, 1968, Physical methods in Advanced Inorganic Chemistry, JohnWiley.
7. K. Burger, 1973, Coordination Chemistry, Experimental methods, Butterworths.
8. C.N.R. Rao, J.R. Ferraro, 1970, Spectroscopy in Inorganic Chemistry, Vol. I and Vol. II, Academic Press.
9. G. Aruldas, Molecular Structure and Spectroscopy, Prentice Hall.

ENVIRONMENTAL CHEMISTRY

Objectives
To know the importance of Environment and methods to save our earth from pollution. To learn more about our earth and environment and how to protect our environment.

Unit I: Environment
1.1 Introduction, composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, biogeochemical cycles of C, N, P, S and O and biodistribution of elements.

Unit II: Hydrosphere
2.1 Chemical composition of water bodies – lakes, streams, rivers and wet lands etc., and hydrological cycle.
2.2 Aquatic pollution – inorganic, organic, pesticide, agricultural, industrial, sewage, detergents and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chlorides, sulphate, phosphate, nitrate and micro-organisms. Water quality standards.

Unit III: Soils and Atmosphere
3.1 Soils - composition, micro and macro nutrients. Pollution – fertilizers, pesticides, plastic and metals. Waste treatment.
3.2 Atmosphere – chemical composition of atmosphere – particles, ions, radicals and their formation.
3.3 Chemical and photochemical reactions in atmosphere: smog formation, oxides of N, C, S and O and their effects. Pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons, green house effect, acid rain, air pollution control and dye chemistry.
3.4 Noise pollution.

Unit IV: Industrial pollution
4.1 Cement, sugar, distillery, paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers and drugs etc. Radionucleide analysis. Disposal of waste and their management.

Unit V: Environmental toxicology
5.1 Chemical remedy to environmental problems, biodegradability, principles of decomposition, Better industrial processes, Bhopal gas tragedy, Chernobyl, three mile island, Sewozo and Minamata disasters. Toxicity of metals – Cd, Hg, Cr, Cu and Pb.

Recommended Books:-
1. Environmental chemistry – S.E. Manahan, Lewis Publishers.
2. Environmental chemistry – Sharma and Kaur, Krishna Publishers.
3. Environmental chemistry – A.K. De, Wiley – Eastern Publishers.
4. Environmental pollution analysis – S.M. Khopkar, Wiley – Eastern Publishers.
5. Environmental toxicology – ED. J. Rose, Gordon and Breach Science Publications.
6. Standard methods of chemical analysis – F.J. Welcher Vol. III, Van Nostrand Reinhold Co.

7. Elemental analysis of air borne particles – Ed. S. Landsberger and M. Greatchman, Gordon and Breach Science Publications.
8. Environmental chemistry – C. Baird, W.H. Freeman.
9. Chemistry of our environment – R.A. Home.

POLYMER CHEMISTRY

Objectives
To know about various types of polymers and their properties. Application of the polymer in the present context and its biodegradation is included.

Unit I: Methods of polymerization

1. Basic concepts of polymer chemistry: Repeating unit, degree of polymerisation, classification, stereochemistry of polymers and nomenclature of stereoregular polymers.
2. Chain, free radical, ionic and ring opening polymerizations. Ziegler – Natta catalyst involment in step polymerisation ring opening polymerisation.
3. Copolymerisation: Block and graft copolymers – preparation.

Unit II: Properties of polymers

2.1 Polymerisation techniques: Bulk, solution, suspension and emulsion polymerisation. Melt, solution and interfacial polycondensation. Solid and gas phase polymerisation.
2.2 Molecular weight and size: Number and weight average molecular weights. Polydispersity and molecular weight distribution in polymers, the practical significance of polymer molecular weights and size of polymers. (Molecular weight determination is not required)
2.3 Glass transition temperature: Concept, associated properties and determination. Glassy solids and glass transition. Factors influencing it.
2.4 Crystallinity in polymers: Polymer crystallisation, structural and others factors affecting crystallisability and effect of crystallinity on the properties of polymers.

Unit III: Resins and plastics

3.1 Processing: Calendering, die casting, rotational casting. Compression, injection, blow and extrusion moulding. Thermoforming, foaming and reinforcing techniques.
3.2 Synthetic resins and plastics: Manufacturing and applications of polyethylene, PVC, teflon, polystyrene, polymethylmethacrylate, polyurethane, phenol – formaldehyde resins, urea – formaldehyde and melamine – formaldehyde resins and epoxy polymers.

Unit IV: Synthetic fibers and rubbers

4.1 Synthetic fibers: Rayon, nylons, polyesters, acrylics, modacrylics and spinning techniques.
4.2 Synthetic rubber: SBR, butyl rubber, nitrile rubber, neoprene, silicone rubber and polysulphides.
4.3 Conducting polymers and applications.

Unit V: Degradation of polymers

1. Polymer degradation: Types - thermal, mechanical, photo, hydrolytic and oxidative degradations.
1. Additives for polymers: Fillers, plasticisers, thermal stabilizers, photo stabilizers, antioxidants and colourants.
2. Biodegradable Polymers and their applications.

References

1. Michael L. Berine – Plastics Engineering Hand Book, 5th Edn. Chapman & Hall, New York, 1991.
2. Jacqueline. I Kroschwitz – concise encyctopedia of polymer science and engineering John Wiley & sons, New York 1998.
3. R.W. Iyson – specialty polymers, blackie academic & professional, London, 19992.
4. Fred.W.Bill mayer, Textbook of polymer science, Third edition, John wiley & sons , Reprint 2013
5. Mourice Morton – Rubber Technology, Van Nostrand, Reinhold New York, 1987.

Elective Paper I

216CMPE01 - ANALYTICAL CHEMISTRY PRACTICALS - I

Objectives

To carry out colorimetric analysis to estimate Fe, Ni, Mg and Cu and to get knowledge regarding chromatographic techniques. To learn the interpretation of spectra of standard organic and inorganic compounds.

I. Colorimetric analysis

Spectrophotometric method: Estimation of iron, nickel, manganese and copper.

II. Chromatographic separations

1. Separation of a mixture of two metal ions by paper chromatography.
2. Separation of zinc and magnesium on an anion exchanger
3. Separation of green leaf pigments by thin layer chromatography
4. Separation of o and p-nitro phenols by column chromatography

III. To learn the basic principles - Extraction of organic compounds from natural source.

1. Caffeine from tea leaves
2. Lactose from milk
3. Citric acid from lemon
4. Pipierine from black pepper
5. Lycopene from tomatoes

Text Books:-

1. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern Limited.
2. Mann and Saunders, Laboratory Chemistry manual of Organic compounds.
3. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.

Elective Paper II

216CMPE02 - PHYSICAL CHEMISTRY PRACTICALS I

Objectives

To understand and verify the principles and theory of physical chemistry experiments. A minimum of 8 experiments have to be performed.

1. Study of the adsorption of acetic acid or oxalic acid on charcoal, verification of Freundlich isotherm and determination of concentration of given acid
2. Construction of phase diagram for a simple binary system; naphthalene – biphenyl, naphthalene –p-dichlorobenzene, naphthalene-diphenylamine.
3. Determination of partition coefficient, equilibrium constant and unknown concentration of potassium iodide of the reaction between iodidine and potassium iodide by partition method.
4. Determination of molecular weight of benzoic acid in benzene and the degree of association of benzoic acid in benzene using partition method.
5. Kinetic study and comparison of rate constants of different acids or acids of different strength for the inversion of cane sugar by polarimetric method.
6. Kinetic study of the reaction between acetone and iodine in acidic medium and determination of the order with respect to iodine and acetone
7. Saponification of ethylacetate by sodium hydroxide and determination of order of the reaction.
8. Comparison of acid strengths for hydrolysis of methylacetate catalyzed by acids
9. Determination of temperature coefficient and energy of activation for the acid catalysed hydrolysis of methylacetate.
10. Determination of the rate constant and order for the reaction between potassium persulphate and potassium iodide
11. Study of the primary salt effect on the kinetics of oxidation of iodide by persulphate
12. Kinetic study of the decomposition of sodium thiosulphate by mineral acid.

References

1. Arthur I. Vogel, A Text Book of Practical Organic Chemistry.

2. V K Ahluwalia etal sunita Dhingra Adarsh Gulati, College Practical Chemistry, 2008

Semester III

316CMPT01 - ORGANIC CHEMISTRY – III

Objectives

The first part of the paper explains the instrumental methods and their application in the determination of structure of organic molecules. The second part includes the basic concepts of aromaticity and photochemistry. A detailed account of orbital symmetry which forms the basis of many organic reactions is also included. The last part of the subject deals with heterocyclics, terpenoids and steroids.

Unit I: Physical methods of structure determination

Principles and applications of ultraviolet and infrared spectroscopy in organic molecular structure determination. Mass spectrometry and its applications. Optical rotatory dispersion and its applications. Cotton effect, Octant rule and axial haloketone rule. Problem solving approach. (for molecules with a maximum number of C_{10}) Woodward Fieser Rule (only applications).

Unit II: NMR Spectroscopy

Nuclear magnetic resonance spectroscopy. Proton chemical shift, spin-spin coupling, coupling constants and applications to organic structures-FT NMR ^{13}C NMR Spectroscopy (elementary treatment). Nuclear overhauser effect (applications only)

Unit III: Organic Photochemistry and Aromaticity

Aromaticity of benzenoid, non-benzenoid and heterocyclic compounds, Huckel's rule-Aromatic systems with pielectrons - numbers other than six non-aromatic (cyclooctatetraene etc) and anti-aromatic systems (cyclobutadiene etc)- with more than 10 pi electrons – Annulenes up to C_{18} (synthesis not expected).

Photo chemistry of ketones, photo oxygenation, photo reduction, photocycloaddition, Paterno - Buchi reaction, Di –pi- methane rearrangement. cis- trans isomerisation, Barton reaction, photo-Fries reaction, photochemistry of cyclohexadienones synthesis of Vit - D.

Unit IV: Orbital symmetry and correlation

Pericyclic reactions-classification, electrocyclic, cycloaddition reactions. Woodword Hoffman rules, FMO-Analysis of electrocyclic, cycloaddition and sigmatropic reactions-correlation diagram for cycloaddition reaction ($\square^{2s}$ + $\square^{2s}$) and ($\square^{4s}$ + $\square^{2s}$) – butadiene – cyclobutene system and Inter conversion of hexatriene to cyclohexadiene. Structure of bulvalene, a fluxional molecule- MO treatment on Cope, Claisen rearrangements, Diels-Alder and Ene reaction.

Unit V: Heterocyclic compounds, Terpenoids and Steroids

Flavones, isoflavones, anthocyanins (Synthesis of parent and simple alkyl or aryl substituted derivatives are expected). Synthesis of carotenoids, licopenes and Vitamin A1 (Reformatsky and Wittig reaction methods only).

Structural elucidation of cholesterol (by chemical degradation). Conversion of cholesterol to progestrone, esterone and testosterone.

Text Books:-

1. R.M. Silverstein, G.C. Bassler and Morril, 1991, Spectrometric identification of Organic Compounds, 5th Edition, John Wiley and Sons, New York.
2. I.L. Finar, 1986, Organic Chemistry – Vol.II, 5th edition, ELBS Publication.
3. P.S. Kalsi, 2002, Spectroscopy of Organic Compounds, Wiley Eastern Ltd, Chennai.
4. H. Depuy and Orville, Molecular reaction and Photochemistry Charles, L.Chapman, Prentice Hall of India Pvt. Ltd., New Delhi
5. L.A. Pacquette, 1978, Principles of Modern Heterocyclic Chemistry, Benjamin Cummings Publishing Co., London.
6. J. March, 1992, Advanced Organic Chemistry, 4th Edition, Singapore
7. F.A. Carey and R.J. Sundberg, 1990, Advanced Organic Chemistry, 4th Edition, Plenum Press, New York.
8. Neil S. Issacs, 1987, Physical Organic Chemistry, ELBS Publication.
9. P.S. Kalsi, 1999, Texbook of Organic Chemistry, Mcmillan India Ltd.

Websites:-

1. http :// info dome. sdsu, ./research/ guides/ science/ org chemistryblr. html
2. http :// www.liv.ac.uk/chemistry/links /reactions.html
3. http ://orgchem.chem..uconn.edu/namereact/named.html
4. www.gcocities.com/ chempen softwar4ee/reactions.html

316CMPT02 - INORGANIC CHEMISTRY – III

Objectives
To understand the applications of different spectroscopic methods in the study of Inorganic compounds.

Unit I: IR and Raman Spectra Application
Effect of coordination on ligand bands- Ammine, Nitro, nitrito, thiocyanato.
Urea complexes, dithiocarbamato complexes, carboxylate complexes, nitrosyl complexes, cyano complexes- nitrate, sulphate and perchlorate complexes- differentiation of geometric isomers. Metal carbonyls, olefin complexes, sandwich complexes.
Raman spectroscopy of metal complexes, organometallic and simple inorganic compounds with special reference to coordination sites, isomerism.

Unit II: Electronic Spectra application
Classification of Transitions – Selection Rules – Free ion terms – Racah Parameter – Ligand field perturbations on the free ion terms – Spectra of Octahedral complexes:d^n configurations- Weak field and strong field ligands – Orgel and Tanabe-Sugano Diagrams – Evaluation of $10D_q$ – Spectra of distorted octahedral complexes – Jahn-Teller Distorion – Tetrahedral Complexes - Nephelauxetic effect – Charge Transfer Spectra.

Unit III: NMR, NQR and Mossbauer
NMR, NQR, Mossbauer spectra: NMR spectra of ^{31}P, ^{19}F, NMR shift reagents, NQR-Nitrosyl compounds. Mossbauer of Fe and Sn systems.

Unit IV: Application of ESR and Photo electron spectroscopy to coordination complexes
ESR introduction-Zeeman equation, g value, nuclear hyperfine splitting, Interpretation of ESR spectrum of simple carbon centered free radicals. Anisotropy in g value and hyperfine splitting constant. McConnels equation, Kramer's theorem, esr of transition metal complex of copper, manganese and vanadyl complexes.
Photoelectron spectroscopy – UPS and XPS-Photoelectron spectra – Koopman's theorem,-Fine structure in PES, Chemical shift and Correlation with electronic charges.

Unit V: X-ray diffraction and Microscopy application
Basic Principles of diffraction – Bravis Lattices- Use of X-ray power diffraction data in identifying inorganic crystalline solids. Single crystal diffraction in crystal structure analysis. Optical Microscopy, Electron Microscopy – SEM and TEM. X-ray Flourescence Spectroscopy – structure determination.

Text Books:-

1. L.Smart, E.Moore – Solid State Chemistry – An Introduction-2nd Edition
2. A.R.West – Basic Solid state Chemistry 1961 – John Wiley
3. A.R.West – Solid state Chemistry and its applications 2007 – John Wiley
4. W.E Addison, 1961, Structural principles in Inorganic Chemistry, Longman
5. Structural principles in inorganic Chemistry –Adams
6. Physical methods in inorganic Chemistry – Russel Drago

7. Physical methods in inorganic Chemistry – E.A.V Ebsworth, Rankin and Caddock. 1987.
8. Vibrational Spectroscopy Theory and Applications – New Age, D.N.Sathyanarayana, 2011.
9. Magenetic Resonance Spectroscopy-ESR, NMR, NQR-IK International D.N. Sathyanarayana, 2014.

References:-

1. R.B.Heslop and K.Jones, inorganic Chemistry, Elsevier Scintific Publ .1976.
2. H.A.O Hill and P.Day, physical methods in dvanced Inorganic Chemistry, John wiley 1968.
3. C.N.R Rao, J.R.Ferraro, Spectrosopy in inorganic chemistry, Vol.I and Vol II, Academic press, 1970.
4. G.Aruldhas, molecular structures and spectroscopy-Prentice hall.
5. M.F.Lappert –Physical inorganic Chemistry-inorganic Electron Spectrosopy 1968.

316CMPT03 - PHYSICAL CHEMISTRY – III

Objectives

To understand and appreciate the significance and applications of classical thermodynamics, electrochemistry in solutions and to learn the principle and applications of optical and resonance spectroscopy.

Unit I: Thermodynamics - I

Partial molar properties - Partial molar free energy (Chemical potential) - Partial molar volume and partial molar heat content - their significance and determination of these quantities. Variation of chemical potential with temperature and pressure.

Thermodynamics of real gases - gas mixture - fugacity definition - determination of fugacity variation of fugacity with temperature and pressure -thermodynamics of ideal and non ideal binary solutions-dilute solutions-excess functions for non-'ideal solutions and their determination-the concepts of activity and activity coefficients-determination of standard free energies.

Choice of standard states - determination of activity and activity coefficients for non-electrolytes.

Unit II: Spectroscopy - II

Rotational spectroscopy of a rigid rotar – non-rigid rotor-diatomic and polyatomic molecules. Vibrational spectroscopy-harmonic oscillator-anhormonicity –Vibration – rotation spectra of diatomic vibrating molecules selection rules-P,Q and R branches.

Vibrational spectra of polyatomic molecules- fundamental vibrations – normal modes of vibration-overtones, combination and difference bands- Fermi resonance. Raman spectra: Classical theory of Raman effect and molecular polarisability – pure rotational Raman spectra – Vibrational Raman spectra – Rotational fine structure – Rule of mutual exclusion – Polarization of light and Raman effect.

Unit III: Spectroscopy - III

Resonance spectroscopy-Zeeman effect-equation of motion of spin in magnetic fields-chemical shift-spin-spin coupling-NMR of simple AX and AMX type molecules- H^1 , ^{13}C, ^{19}F, ^{31}P NMR spectra - a brief qualitative discussion of Fourier transform spectroscopy. ESR: principle, spin-orbit coupling. Hyperfine interaction. McConnell reactions.

Mass spectra: Theory and instrumentation, McLaffetry rearrangement fragmentation pattern for simple aliphatic and aromatic alkanes, alcohols, aldehydes and ketones.- Mossbauer spectroscopy-Doppler effects, isomer shift, electron-neutron hyperfine interactions. Quadrupole interactions and Magnetic interactions.

Unit IV: Electrochemistry of solution

Mean ionic activity and activity coefficient: concept of ionic strength, Debye-Huckel theory of strong electrolytes-activity coefficient of strong electrolytes-determination -Debye Huckel limiting law at appreciable concentration of electrolytes - Debye Huckel Bronsted equation-qualitative and quantitative verification.

Redox reaction: cell potential, Galvanic cell, Electrolytic cell, Nernst equation for cell potential of electrolyte. Electrode equilibrium-thermodynamic electrodes and electrode potential, electrochemical cells and electromotive force.

Unit V: Quantum Chemistry – IV

Approximation methods –perturbation and variation method –application to hydrogen ,helium atoms –R.S. coupling and term symbols for atoms in the ground state – Slater orbital and HF –SCF methods Born – Heimer approximation –valence bond theory for hydrogen molecule –LACO –MO theory for di and polyatomic molecules –concept of hybridization – Huckel theory for conjugated molecules (ethylene , butadiene and benzene)- semi empirical methods .

Text Books

1. S. Glasstone, 1960, Thermodynamics for chemists, Affiliated East West Press, New Delhi.
2. J. Rajaram and J.C. Kuriacose, 1986, Thermodynamics for students of chemistry, Lal Nagin Chand, New Delhi.
3. A. Caringtion and A.D Mc Lachlan, 1967, Introduction to Magnetic Resonance
4. Harper and Row, New York.
5. G. Aruldas, 2002, Molecular structure and spectroscopy, Prentice Hall.
6. C.N. Banwell, 2003, Fundamentals of Molecular, Spectroscopy Tata McGraw Hill.
7. D.N. Sathyanarayana vibrational spectroscopy
8. D.N. Sathyanarayana electronic spectroscopy
9. J.O.M. Bokris and A.K.N. Reddy, 1977, Electrochemistry, VoIs1 and 2 Plenum, New York..
10. J. Robbins -1993, Ions in Solution-An Introduction in electrochemistry, Clarendon press, Oxford
11. R.K.Prasad, 1992, Quantum Chemistry, Wiley Eastern, New Delhi.
12. D.A. Mcquarrie, 1983, Quantum Chemistry, University Science Books, Mill Valley, Calfornia.

Suggested Reference Books

1. R.L. De Koch and H.B. Gray, Chemical Structure and Bonding, Benjamin/Cumming, Menlo Park, California.
1. J.N. Murrell, S.F.A. Kettle and J.M. Tedder, 1985, The Chemical Bond, Wiley.
2. P.W. Atkins, 1983, Molecular Quantum Mechanics, Oxford University Press, Oxford.
3. P.H. Rieger, 1994, Electrochemistry, Chapman and Hall, New York.
4. W. Kemp, 1986, NMR in Chemistry McMilan Ltd.
5. G.W. King, 1964, Spectroscopy and Molecular Structure, Holt Rieneheart and
6. Winston.
7. K.D. Mclauchlan, 1970, Magnetic Resonance, Oxford chemistry Series, Oxford.
8. B.P.Staughan and S.Walker, 1976, Spectroscopy Vol. 1 , 11 and 111, Chapman and
9. Hall.
10. B.W. Cook and K. Jones, 1972, A.Programmed Introduction to Infra red
11. spectroscope, Heydon and Son Ltd.
12. F.A. Rushworth and D.P Tunstal, 1973, Nuclear Magnetic Rewsonance Gorden and Breaqch Science Publishing, New York.
13. J.K. Sanders and B.K.Hunther, 1987, Mordern NMR Spectroscopy, A Guide for Chemists, Oxford University Press, Oxford.
14. J.K.M. Sanders, E.C. Constable and B.K. Huntherm Morden, 1989, NMR
15. Spectroscopy - A World Book of chemical problems, Oxford.

EXTRA DISCIPLINARY ACTIVITY – II

316CMPT04

MATERIALS SCIENCE

Objectives

The objective is to give precise account of synthesis of materials and their magnetic and electrical properties. Solid state analysis and crystal defects in solids are also included.

Unit I: Solid state analysis

1.1 Structure and bonding in solids-cohesive forces in crystals-van der waal's interactions, ionic, covalent and hydrogen bonding in solids.

1.2 Techniques of structure determination in solid state- X-ray diffraction, electron and neutron diffractions and electron microscopy: principle, instrumentation and applications.

Unit II: Crystal defects in crystals

1.1 Theories of metallic state- free electron theory, Brillouin and Band models.

1.2 Smart metals – binary and ternary – examples and applications.

1.3 Defects in crystals-Frenkel and Schotky defects, f centers, effect of defects on the electrical, optical, magnetic, thermal and mechanical properties.

Unit III: Conducting materials

3.1 Optimized ionic conductors – silver ion, copper ion, alumina and related electrolytes, alkali metal ion and fluoride ion and proton conductors- super conductors- principle and applications.

3.2 Photoconducting materials- principle and applications.

Unit IV: Electrical properties of materials

4.1 Charge transfer complexes-characterization and their electrical properties.

4.2 Conducting polymers – polyacetylenes, polyanilines and polyvinylidenes – preparation and applications.

4.3 Liquid crystals – classification-thermotropic and lyotropic –nematic, smectic and cholesteric crystals and their applications.

Unit V: Synthesis of nano materials

5.1 Preparation and properties of nanoparticles –Materials-metals, semiconductors, ceramics (oxides, carbides, sulphides, nitrides)-Physical methods: vapour deposition(evaporation and sputtering) –chemical methods: reduction and sol-gel methods. optical properties ,electrical properties and magnetic properties

5.2 Carbon nano structures: carbon clusters, C_{60}- alkali doped C_{60}- carbon nanotubes - preparation- arc-discharge, laser ablation and catalytic decomposition of hydrocarbons-electronic and mechanical properties- applications – field emission. Sensors- mechanical reinforcement.

References

1. Materials Science – Raghavan
2. Materials Science - Manas Chanda Vol I &II
3. A.F.Wells, 1984, Structural Inorganic Chemistry, V.Edition, Oxford.

4. A.R. West, Solid State Chemistry and applications 1991, John Wiley
5. Lesley Smart and Elaine Moore, Solid State Chemistry,
6. Kenneth, J. Klabunde, Nanoscale materials in chemistry, Wiley Interscience, 2001
7. T . Pradeep , Nano : The Essentials ,Tata McGraw-Hill Publishing Company Limited, 2007.
8. Sulabha K. Kulkarni, Nano technology, Principles and practices, Capital publisher 2007.

BIOORGANIC CHEMISTRY

Objectives

This course aims to explain the basic concepts in chemistry and metabolism of carbohydrates, amino acids, proteins and lipids. In addition the student can gain the understanding of various types of nucleic acids and classification of vitamins and enzyme.

Unit I: Chemistry and metabolism of carbohydrates

Definition, classification and biological role of carbohydrates.

Monosaccharides linear and ring structures (Haworth formula) of ribose, glucose, fructose and mannose (structural determination not required) physical and chemical properties of glucose and fructose.

Disaccharides: Ring structures (Haworth formula) - occurrence, physical and chemical properties of maltose, lactose and sucrose.

Polysaccharides: Starch, glycogen and cellulose - structure and properties.

Glycolysis of carbohydrates.

Unit II: Chemistry and metabolism of Amino acids and Proteins

Amino acids: Various classifications, essential amino acids, physical properties (amphoteric nature and isoelectric point) and reactions.

Proteins: Classifications (based on shape, composition and solubility), physical properties.

Primary structure - End group analysis (N- terminal analysis- Edman's method, dansyl chloride method; C - terminal analysis- hydrazinolysis and bio - chemical methods)

Biological functions of proteins, Deamination, transamination reactions, Urea cycle.

Unit III: Chemistry and metabolism of Lipids

Definition, classification- simple lipids (fatty acids), compound lipids and derived lipids. Properties: saponification number and acetyl number.

Cholesterol (structure elucidation not needed), biological importance and chemical properties. Bile acids- functions. Biological functions of lipids.

Unit IV: Nucleic acids

Purine and pyrimidine bases, nucleosides, nucleotides, polynucleotides, various types of DNA and RNA structures.

Biological functions of DNA and RNA. Genetic code.

Unit V: Vitamins

Vitamins: Definition, classification- water-soluble vitamins (B_v B_2, B_3, B_6, B_{12} and vitamin-C) and fat-soluble vitamins (A, D, E and K) - occurrence, structure, deficiency diseases, biochemical rules and daily requirements.

Suggested Reference Book

1. Biochemistry C.B. Powar and G.R. Chatwal.
2. Elements of Biochemistry Ragunatha Rao
3. Essential Biochemistry U. Sathyanarayanan
4. Essential Biochemistry J.L. JAIN

RESEARCH METHODOLOGY

OBJECTIVES

The aim is to explain various aspects of research methodology- Literature, planning, data analysis and report writing.

UNIT I: Research Problem

1.1 Objectives of research, types of research – basic, applied, and other types.
1.2 Problem selection – project proposal - funding agencies.

UNIT II: Source of Literature

1.3 Chemistry literature survey –primary, secondary and tertiary sources.
2.2 Journals published by the ACS and RSC – CA and its importance –Indian Journals – reviews, monographs, data books and indexes.
2.3 Methods of searching, compilation, preservation and retrieval of collected literature.
1.1 Impact factor and citation index.

UNIT III: Research planning, methods and materials

1.1 Planning and conducting experiments.
1.2 Methods of collecting data – primary and secondary –sources of secondary data.
1.3 Classification and tabulation of data – types of classification –general rules for tabulation– types of tables.
1.4 Simple sampling techniques and size of the sample.

UNIT IV: Analysis of data

4.1 Presentation of data - Types of errors – Gross, systematic and random errors.
4.2 Measures of central tendency, mean, standard deviation and measures of variability.
4.3 Linear regression, correlation and method of least squares.

UNIT V: Report writing

5.1 Project report writing – general, chapter and page format.
5.2 Procedure for presenting tables, graphs and figures, foot-notes, bibliography and appendices.
5.3 Abbreviations, symbols and SI units.
5.4 Plagiarism, copy right and patent laws.
5.5 Publication of research paper.

Suggested Reference Books

1. Thesis and Assignment Writing – J Anderson, B.H. Dursten and M. Poole, Wiley Eastern (1977).
2. Statistical Method, Gupta S. P, Sultan Chand and Sons, New Delhi, 2004
3. Hand Book for Authors –Journal of the American Chemical Society Publications
4. Chemical publications – Their nature and uses

BIOINORGANIC CHEMISTRY

Objectives

The aim of this elective is to explain the basic biological concepts, Enzyme catalysis, importance of trace elements and photo synthesis. Further the concept of bio analytical chemistry is discussed.

Unit I: Basic biological concepts

Thermodynamics and biology – Basic concepts of structure and functionality – membranes – structure, function, transport properties, aspects of electrochemical phenomena – active transport, ionophores, biological energy storage and Phosphate hydrolysis.

Unit II: Enzymes catalysts

Enzymes - Nomenclature and classification, the free energy of activation, the effects of catalysts and kinetics of enzyme catalysed reactions – Michelis - Menton equation - Effect of pH and temperature. Factors affecting to the catalytic efficiency. Spectroscopic methods.

Unit III: Essential of trace metal ions

Coenzymes - Vitamin B_{12} coenzymes, carboxypeptidase and Superoxide dismutase.
Heme-enzyme - Peroxidase and catalases.
Oxygen carriers - Hemeproteins - Haemoglobin, myoglobin – Structure, oxygenation and stereochemistry - Bohr effect. Non-heme oxygen carriers - Hemerythrin and hemocyanin.

Unit IV: Nitrogen fixation and Photosynthesis

Nitrogen fixation - Introduction, types of nitrogen fixing micro organisms. nitrogenase enzyme - Metal clusters in nitrogenase - redox property - Dinitrogen complexes - transition metal complexes of dinitrogen - nitrogen fixation via nitride formation and reduction of dinitrogen to ammonia.
Biological redox systems: Cytochromes -Classification, cytochrome a, b and c. Cytochrome P-450.
Iron - sulphur proteins - rubredoxin and ferredoxin.
Role of chlorophyll in photosynthesis

Unit V: Bioanalytical Chemistry and Metals in Medicine

Toxicity & medicine.
Toxicity of Hg, Cd, Zn, Pb, As, Sb.
Anti cancer agents.
Metals for Diagnostic and chemotherapeutic purposes (B, Au, Gd, Li, Tc, Pt, Ru).
Metal ion poisoning: Failure of metal ion control systems and role of metal ion.
Diagnosis and treatment – anticancer agents.
Pollution studies: Effluents and treatment.
Inorganic plant nutrition and indicator plants for mineral exploration.

Text Books:-

1. Williams, D.R. - Introduction to Bioinorganic Chemistry
2. Fiabre, F.M., and Williams D.R. - The Principles of Bioinorganic Chemistry, Royal Soceity of Chemistry, Monograph for Teachers - 31.
3. Purcell, K.F. and Kotz, J.C., - Inorganic Chemistry
4. Elements of Bioinorganic Chemistry - G.N. Mugherjee and Arabinda Das, 1993.

5. Bioinorganic Chemistry - M. Satake and Y. Mido, Discovery Publishing House, New Delhi (1996).

Reference Books:

1. G. Eichorn, G. - Inorganic Bio-Chemistry Vol. I and II, Elsevier, 1973.
2. J.W. Huheey - Inorganic Chemistry, Harper and Row.
3. Metal ions in Biological Systems, Vol. I to XV, H. Siegel (Ed.)
4. R.W. Hay - Bio Inorganic Chemistry.

Elective Paper III

316CMPE01 - ORGANIC CHEMISTRY PRACTICAL II

Objectives

To prepare the following organic compound involving two stages and. Quantitative estimation of organic compounds.

I. Interpretation of organic compounds. (UV, IR, PMR and Mass spectra) -Any 10

1. 1, 3, 5-trimethylbenzene
2. pinacolone
3. prophyl amine
4. p-methoxybenzyl alcohol
5. benzyl bromide
6. phenyl acetone
7. 2-methoxyethyl acetate
8. acetone
9. isopropyl alcohol
10. acetaldehyde diacetate
11. 2-N, N-dimethylamino ethanol
12. pyridine
13. 4-picoline
14. 1, 3 dibromo-1, 1-dichloropropene
15. cinnamaldehyde.

II. Preparation of the following (Any Six):-

1. Sym-Tribromobenzene from aniline.
2. p-nitro aniline from acetanilide
3. m-Nitrobenzoic acid from methyl benzoate.
4. 2, 4-Dinitrobenzoic acid from p-nitro toluene.
5. m-Nitro benzoic acid from benzaldehyde
6. p-bromoaniline from acetanilide
7. Anthraquionone from phthalic anhydride.
8. Phthalide from phthalic anhydride
9. 2-phenyl indole from phenylhydrazine
10. 2-4, Dinitrophenyl hydrazine from p-nitrochlorobenzene.

III. Quantitative estimation of organic compounds-Any 6

1. Estimation of aniline
2. Estimation of phenol
3. Estimation of glucose (Bertrands Methods)
4. Saponification of fat or an oil.
5. Iodine value of an oil.
6. Estimation of Ketone.
7. Estimation of amino group.
8. Estimation of amide group
9. Estimation of sulphur in an organic compound.

Recommended Books:-

1. Arthur I. Vogel, A Text Book of Practical Organic Chemistry.
2. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern Limited.
3. Mann and Saunders, Laboratory manual of Organic Chemistry

Elective Paper IV

316CMPE02 - INORGANIC CHEMISTRY PRACTICAL II

OBJECTIVES

To acquire skill in preparation of coordination complexes and to estimate gravimetrically and volumetrically the given metals ions (Mg, Ni, Zn, Fe and Cu) in the given mixture and analysis of ores and alloys.

Unit I: Preparation of the following:-Any 5

1. Sodium bis(thiosulphato)cuprate (I)
2. Sodium hexanitrocobaltate (III)
3. Chloropentammine cobalt (III) chloride
4. Bis (acetylacetanato) copper (II)
5. Hexaminenickel (II) chloride
6. Bis (thiocynato) pyridine manganese, (II)

Unit II: Quantitative analysis: Mixture of metal ions (gravimetrically and volumetrically)

2.1 magnesium and Iron in the mixture of Iron and magnesium
2.2 Nickel and copper in the mixture of copper and nickel
2.3 Zinc and copper in the mixture of copper and zinc.
2.4 Nickel and Iron in the mixture of iron and Nickel.

Unit III: Analysis of Ores and Alloys:-

3.1 Determination of percentage of calcium and magnesium in dolomite.
3.2 Determination of percentage of MnO_2 in pyrolusite.
3.3 Determination of copper and zinc in brass.

Text Books:-

1. Vogel, Text book of Inorganic quantitative analysis.
2. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.

Semester IV

416CMPT01 - ORGANIC CHEMISTRY – IV

Objectives

This paper introduces the basic methodologies for the synthesis of organic compounds. A brief introduction to biosynthesis of alkaloids and terpenoids is also included.

Unit I: Bio-Organic chemistry

Synthesis of Pyrimidines and purines.
Structure and role of nucleic acids. DNA and RNA Genetic code.
Biosynthesis of cholesterol, phenanthrene alkaloids and bile acids.

Unit II: Alkaloids and Proteins

Structural elucidation and total synthesis of morphine.
Peptides and their synthesis (Synthesis of tripeptide using amino acids - Glycine, Alanine, Lysine, Cysteine, Glutamic acid, Arginine).Merrified synthesis, Determination of primary, secondary and tertiary structure of proteins.

Unit III: Modern synthetic methodology

Application of synthetic methodology for the synthesis of simple cyclic and acyclic target molecules -synthesis of cubane, 5 - hexenoicacid , bicyclo (4, 1, 0) heptane-2-one.,trans 9-methyl-1-decalone ,longifolene and onocerin. Concept of Synthones, synthetic equivalents and intermediates. Formation of C-C and C=C bonds. Reversal carbonyl polarity – Umpolung addition.

Unit IV: Retrosynthetic analysis, Protection and Deprotection

Retro synthetic analysis and synthesis of simple organic molecules such as 1,2, 1,3, 1,4 and 1,5 dicarbonyl compounds both acylic and cyclic. Formation of 3, 4, 5 and 6 membered cyclic compounds - Baldwin's rules. Use of standard reactions, like Grignard reactions, Robinson annulations. Protection and deprotection of functional groups (R-OH, RCHO, R-CO-R, R-NH_2 and R-COOH). Use of PTC (Phase-transfer catalyst) and Crown ethers in organic synthesis.

Unit V: Novel reagents in organic synthesis:-

Synthesis and applications of Organolithium, Organomagnesium, Organozinc and Organo Copper and Gilman reagents. Modern synthetic methods: metal mediated C-C coupling reactions: Mechanism and synthetic applications of Heck, Stille, Suznki, Negishi, Sonogashira, McMurray, Metathesis and Carbonylation reactions. Green reactions and reagents.

Text Books:-

1. R.K. Mackie and D.M. Smith. 1998, Guide book to organic synthesis, ELBS Publication.
2. L. Finar, 1986, Organic Chemistry, 5th Edition, Vol .II, ELBS Publication.
3. L. Smith, Robert L. Hill .1. Robert Lehman, Robert J .Iet Rowitz, Philp Handler and abrahim white principles of Biochemistry General aspects, 7th Edition, McGraw Hill Int.
4. L. Stryer, Biochemistry, W.H.Freeman and Co., New York.
5. Agarwal, Chemistry of Organic Natural Products, Goel Publishing House.
6. B.l. Smith, 1980, Organic synthesis, Chapman and Hall, NY.
7. Francis.A. Carey, Richard J. Sundbreg, 2001, Advanced Organic Chemistry, 4th Edition, Plenum Press, New York.

8. N.J. Turro, 1978 Modern Molecular Photochemistry, Benjamin, Cummings, California.

Websites:-

1. http://infodome.sdsu,./research/guides!science!orgchemistryblr.html
2. http://www.liv.ac.uklchemistry/links/reactions.html
3. http://orgchem.chem..uconn.edu/namereacVnamed.html
4. www.gcocities.com/chempensoftwar4ee/reactions.html)

416CMPT02 - INORGANIC CHEMISTRY – IV

Objectives

This paper exposes the student to the importance of metal ions in biology and the chemistry of organometallic compounds and their industrial applications.

Unit I: Bio-Inorganic Chemistry - I

Metal storage, transport and biomineralisation: ferritin, transferrin. Metal ion pumps - sodium and potassium.

Essential and trace metal ions.

Metalloenzymes – Zinc Enzymes, carboxypeptidase and carbonic anhydrase, Vitamin B_{12}, catalase, peroxidase, superoxide dismutase and blue copper proteins.

Unit II: Bio-Inorganic Chemistry – II

Transport Proteins – Oxygen carriers – Haemoglobin, myoglobin – Structure, oxygenation and stereochemistry – Bohr effect, Non-heme oxygen carriers – Hemerthrin and hemocyanin.

Biological redox systems – ruberdoxin and ferrodoxin.

Role of Chlorophylls in photosynthesis

Anti cancer agents, role of metal ion in diagonis and treatment – use of radioisotopes.

Unit III: Organometallic Chemistry

1.1 Carbon donors: Alkyls and aryls, metalation, bonding in carbonyls and nitrosyls, chain and cyclic donors, olefin, acetylene, and allyl systems. Metallocenes: synthesis, structure and bonding.

3.3 Reactions: Association, substitution, addition, elimination, ligand protonation, electrophilic and nucleophilic attack on ligands, carbonylation, decarboxylation and oxidative addition.

Unit IV: Industrial applications of Organo Metallic compounds

Catalysis – Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalyst(Oxo process), oxidation of olefins to aldehydes and ketones(Wacker process):polymerisation(Ziegler-Natta catalyst); Cyclo oligomerisation of acetylene using nickel catalyst(Reppe's catalyst), polymer bound catalysts. Ziegler-Natta catalysis (metallocene and Nom-Metallocene type catalyst).

Unit V: Inorganic Photochemistry

Principles of Inorganic Photochemistry – Photoredox reactions and photosubstitution reactions in coordination complexes with particular reference to Co(III), Cr(III) and Pt(II) complexes. Photosensitisation reactions of [Ru(bpy)3]2+ complex and its applications in solar energy conversions and DSSC's (Dye Sensitized Solar Cells)

Text Books:-

1. N,J,Turro, 1978, molecular photochemistry.
2. K.K.Rohatgi Mukherjee
3. Purcell, K.F. and Kotz, J.C., - Inorganic Chemistry
4. D.F.Shrivers, Atkins.Inorganic Chemistry
5. J.E. Huheey, 1993, Inorganic Chemistry - Principles, Structure and Reactivity; IV Edition, Harper Collins, NY.

6. S. Manku, 1984, Inorganic Chemistry, TMG Co.,
7. Selected Topics in Inorganic Chemistry, U.Malik, G.D.Tuli, R.D.Madan, 1992.
8. Basolo and R.G. Pearson, 1967, Mechanism of Inorganic Reactions, Wiley, NewYork.
9. R.Sarkar, general and Inorganic chemistry, (Parts I and II), New Book Agency, Calcutta

References:-

1. S.F.A. Kettle, 1973, Coordination Chemistry, ELBS
2. G.Coates, M.L.green and K.Wade, Priciples of Organometallic Chemistry, 1988.
3. R.B.Jordan, Reaction Mechanism of Inorganic and Organo Metallic systems – OUP 1991.
4. P.Powell, Principles of Organometakkic chemistry, Chapman and hall 1998.
5. R.C.Mehothra, A.Singh, Organo Metallic Chemistry, Wiley Eastern Comp.2000.
6. V.Balzani & Carrasitti – Photochemistry of coordination compounds.

416CMPT03 - PHYSICAL CHEMISTRY – IV

Objectives

To learn the principles of photophysics and photochemistry and their applications in organic and inorganic chemistry, energy conversion, Principles and applications of statistical thermodynamics and electrode kinetics are also included in this paper.

Unit I: Fundamentals of photochemistry

Absorption and emission of radiation-Franck-Condon Principle- Decay of electronically excited states, Jablonski diagram: radiative and non radiative processes-fluorescence and phosphorescence-spin forbidden radiative transition internal conversion and intersystem crossing- Einstein coefficient, energy transfer process-excimers and exciplexes-static and dynamic quenching-Stern Volmer analysis.

Unit II: Techniques and Photochemical reactions

Quantum yield and life time measurements, Flash photolysis, Principle and its application, Actinometry. Photo physical process and kinetics of photochemical reactions. Radiolysis of molecules of biological interest (Carbohydrates, Amino acids, Peptides and Nucleic acid). Photoredox reactions and photosubstitution reactions in coordination chemistry Photoreduction and photocycloreduction in organic chemistry - photovoltaic and photogalvanic cells. photoelectrochemistry, Aspects of solar energy conversion. Photosensitization and chemiluminescence.

Unit III: Electrode Kinetics

Electrode-electrolyte interface - electrical double layer-electrocapillary phenomena - Lippmann equation-structures of double layers – Stern, Helmholtz –Perrin and Guoy- Chapmann models.

Mechanism of electrode reaction - polarization and overpotential, the Butler - Volmer equation for one step and multistep electron transfer reactions- significance of exchange current density and symmetry factor-transfer coefficient and its significance-mechanism of hydrogen and oxygen evolution reactions.

Corrosion and passivation of metals: Pourbaix and Evans diagrams - fuel cells-electrodeposition – principle, applications and anticorrosion techniques.

Unit IV: Thermodynamics - II

Concept of thermodynamic probability - distribution of distinguishable and non-distinguishable particles .Maxwell-Boltzmann, Fermi-Dirac and Bose Einstein statistics - modes of contribution to energy- Partition function - translational, vibrational and rotational partition functions for mono, diatomic and polyatomic ideal gases.

Thermodynamic functions in terms of partition functions, Sackur-Tetrode equation equilibrium constant for isotope exchange and dissociation of diatomic molecules;

Unit V: Thermodynamics - III

Heat capacity of solids (Einstein and Debye Models) ortho and para hydrogen -Planck's radiation law - electrons in metals.

Non equilibrium processes, entropy production in irreversible processes, microscopic reversibility, linear force and flux relations, Onsager's law, phenomenological equations, Curie's theorem.

Text Books:-

1. J.O.M. Bokris and A.K.N. Reddy, 1977, Electrochemistry, VoIs1 and 2 Plenum, New York.
1. P. Delahay - 1965, Electrode Kinetics and Structure of Double layer, Interscience,
2. New York.
3. S. Glasstone, 1960, Introduction to Electrochemistry, Affiliated East West Press, New Delhi.
4. D.R. Crow, 1991, Principles and Applications of Electrochemistry, Chapman and Hall.
5. N.J. Turro, 1978, Modern Molecular Photochemistry, Benjamin, Cummings, Menlo Park, California.
6. K.K. Rohatgi Mukherjee, 1978, Fundamentals of Photochemistry, Wiley Eastern Ltd.
Gilbert & J. Bagesot, Essentials of Molecular Photochemistry Blackwell Scientific (1990)
7. M.C. Gupta, 1990, statistical; thermodynamics, wiley eastern New Delhi
8. B.J. McClelland, 1973, Statistical Thermodynamics, Chapman and Hall, London.

Suggested Reference Books:-

1. J.G. Calvert and J.N. Pitts, 1966, Photochemistry, Wiley, London.
2. R.P. Wayne, 1970, Photochemistry, Butterworths, London.
3. R.P. Cundell and A. Gilbert, 1970, Photochemistry, Thomas Nelson London.
4. R.HASSE, 'Thermodynamics of Irreversivble processes', Addison Wesley, Reading. Mass, 1989.

PRACTICAL

416CMPP01 - PHYSICAL CHEMISTRY PRACTICALS II

Objectives
To carry out conductometric and potentiometric experiments in order to acquire skill in the determination of equivalent conductance and solubility product etc.

I Conductometric Experiments

1. Determination of equivalent conductance of strong electrolytes and verification of Debye Huckel Onsager equation.
2. Determination of dissociation constant of weak electrolytes by Ostwald dilution law.
3. Conductometric titrations
    a. single and mixture of strong and weak acids against strong base.
    b. single and mixture of halides against silver nitrate.

II Potentiometric Experiments

1. Determination of pH and pKa
2. Determination of solubility product of a sparingly soluble salt.
3. Potentiometric titrations
    a. single and mixture of strong and weak acids and strong base
    b. Redox titrations by emf measurements.
    c. Precipitation titration of mixture of halides.

References

1. Arthur I. Vogel, A Text Book of Practical Organic Chemistry.
2. V K Ahluwalia etal sunita Dhingra Adarsh Gulati, College Practical Chemistry, 2008

PROJECT

416CMPP02 - Dissertation & Viva Voce Exam

Registrar