M.Sc. CHEMISTRY

SYLLABUS : 2012

CHOICE BASED CREDIT SYSTEM (CBCS)

St. JOSEPH'S COLLEGE (Autonomous)

Re-accredited with 'A' Grade (3rd Cycle) by NAAC

College with Potential for Excellence by UGC

TIRUCHIRAPPALLI - 620 002, INDIA.

FEATURES OF CHOICE BASED CREDIT SYSTEM

PG COURSES

The Autonomous (1978) St. Joseph's College, accredited with Five Star status in 2001, Re-accredited with **A⁺ Grade** from **NAAC (2006),** Re-accredited with **A Grade** from **NAAC (3rd cycle)**, had introduced the Choice Based Credit System **(CBCS**) for PG courses from the academic year 2001-2002. As per the guidelines of Tamil Nadu State Council of Higher Education (TANSCHE) and the Bharathidasan University, the College has reformulated the CBCS in 2008-2009 by incorporating the uniqueness and integrity of the college.

OBJECTIVES OF THE CREDIT SYSTEM

- To provide mobility and flexibility for students within and outside the parent department as well as to migrate between institutions
- To provide broad-based education
- To help students learn at their own pace
- To provide students scope for acquiring extra credits
- To impart more job oriented skills to students
- To make any course multi-disciplinary in approach

What is credit system?

Weightage to a course is given in relation to the hours assigned for the course. Generally one hour per week has one credit. For viability and conformity to the guidelines credits are awarded irrespective of the teaching hours. The following Table shows the relation between credits and hours.

Sem.	Specification	No. of Papers	Hour	Credit	Total Credits
I – IV	Core Courses (Theory & Practical)	14	6	14 x 5	70
	Project	1	--	1 x 5	05
I – IV	3 – Core Electives 1 – Soft Skill Course (Common) (IDC-1)	3	4	3 x 4	12
	1 – Inter Dept. Courses (IDC-2)	2	4	2 x 4	08
I – IV	SHEPHERD – Extension Activity	~	70	5	05

Total Minimum Credits **100**

Other Additional Credits (Dept. Specific) **....**

However, there could be some flexibility because of practicals, field visits, tutorials and nature of project work.

For PG courses a student must earn a minimum of 100 credits. The total number of courses offered by a department is 20. However within their working hours a few departments can offer extra credit courses.

Course Pattern

The Post Graduate degree course consists of three major components. They are Core Course, Elective Course and Inter Departmental Course (IDC). Also 2 compulsory components namely Project / Project related items and SHEPHERD, the extension components are mandatory.

Core Course

A core course is the course offered by the parent department, totally related to the major subject, components like Practicals, Projects, Group Discussions, Viva, Field Visits, Library Record form part of the core course.

Elective Course

The course is also offered by the parent department. The objective is to provide choice and flexibility within the department. The student can choose his/her elective paper. Elective is related to the major subject. The difference between core course and elective course is that there is choice for the student. The department is at liberty to offer three elective courses any semester. It must be offered at least in two different semesters. The staff too may experiment with diverse courses.

Inter Departmental Course (IDC)

IDC is an inter departmental course offered by a department for the students belonging to other departments. The objective is to provide mobility and flexibility outside the parent department. This is introduced to make every course multi-disciplinary in nature. It is to be chosen from a list of courses offered by various departments. The list is given at the end of the syllabus copies. Two IDC s must be taken by students which are offered in Semester II & III. In

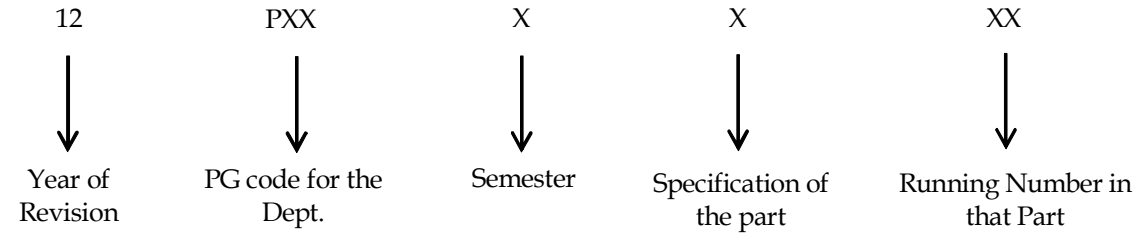
semester II, a common IDC, Soft Skills is to be offered by JASS (Joseph Academy of Soft Skills).

Day College (Shift-I) student may also take an IDC-2 from SFS (Shift-II) course and vice versa

The IDC are of application oriented and inter-disciplinary in nature.

Subject Code Fixation

The following code system (9 characters) is adopted for Post Graduate courses:



01 – Core Courses: Theory & Practical
02 – Core electives
03 – Additional Core Papers (if any)
04 – Inter Departmental Courses
05 – Project
06 – SHEPHERD

CIA Components

The CIA Components would comprise of two parts: (1) Test Components conducted by Controller of Examination (COE) and (2) Teacher specific component. The two centralized tests will be conducted by the COE (Mid-Semester Test & End-Semester Test) for 30% each administered for 2 hours duration. The remaining 40% would comprise of any three components as listed below and will be carried out by the faculty concerned for that paper.

* Assignment, Quiz (Written / Objective), Snap Test, Viva-Voce, Seminar, Listening Comprehension, Reading Comprehension, Problem Solving, Map Reading, Group Discussion, Panel Discussion, Field Visit, Creative Writing, Open Book Test, Library Record, Case Study, etc.

* As a special consideration, students who publish papers in referred journals would be exempted from one of the teacher specific internal components in one of the papers. At the beginning of each semester, the four internal components would be informed to the students and the staff will administer those components on the date specified and the marks acquired for the same will be forwarded to the Office of COE.

Evaluation

For each course there are formative continuous internal assessment (CIA) and semester examinations (SE) in the weightage ratio 50:50.

Once the marks of CIA and SE for each course are available, the Overall Percentage Mark (OPM) for a student in the programme will be calculated as shown below:

$$OPM = \frac{\sum_i C_i M_i}{\sum_i C_i}$$ where C_i is the credit earned for that course in any semester and M_i is the marks obtained in that course.

The Scheme of Over-all Results is as follows:

	PG	
Class	**Arts (OPM)**	**Science (OPM)**
SECOND	50 to 59.99	50 to 59.99
FIRST	60 to 74.99	60 to 79.99
DISTINCTION	75 & Above	80 & Above

Declaration of Result

Mr./Ms. _____ has successfully completed M.Sc./M.A. degree course in _____. The student's overall average percentage of marks is _____ and has completed the minimum 100 credits. The student has also acquired _____ (if any) additional credits from courses offered by the parent department.

M.Sc. Chemistry - Course Pattern - 2012

Sem.	Code	Course Title	Hrs/Wk	Credits
I	12PCH1101	Organic Chemistry I	6	5
	12PCH1102	Inorganic Chemistry I	6	5
	12PCH1103	Physical chemistry I	6	5
	12PCH1104	Organic Chemistry Practical I	4	3
	12PCH1105	Physical Chemistry Practical I	4	3
	12PCH1201A 12PCH1201B	Core Elective I **A:** Analytical and photo chemistry **B:** Organometallic Chemistry (or)	4	4
		Total for Semester I	**30**	**25**
II	12PCH2106	Organic Chemistry II	6	5
	12PCH2107	Inorganic Chemistry II	6	5
	12PCH2108	Physical chemistry-II	6	4
	12PCH2109	Organic Chemistry Practical II	4	3
	12PCH2110	Physical Chemistry practical-II	4	3
	12PSK2401	IDC – I: Soft Skills	4	4
		Total for Semester II	**30**	**24**
III	12PCH3111	Organic Chemistry III	6	4
	12PCH3112	Inorganic Chemistry III	6	5
	12PCH3113	Physical Chemistry-III	6	5
	12PCH3114	Inorganic Chemistry Practical I	4	3
	12PCH3202A 12PCH3202B	Core Elective II A: Natural Products B: Pharmaceutical Chemistry (or)	4	4
	12PCH3402	IDC – II: Health Chemistry	4	4
		Total for Semester III	**30**	**25**
IV	12PCH4115	Organic Chemistry IV	4	3
	12PCH4116	Inorganic Chemistry IV	4	3
	12PCH4117	Physical Chemistry IV	4	3
	12PCH4118	Inorganic Chemistry Practical II	4	3
	12PCH4203A 12PCH4203B	Core Elective III A: Application of Thermodynamics and Electrochemistry B: Thermodynamics (or)	4	4
	12PCH4501	Project	10	5
		Total for Semester IV	**30**	**21**
I– IV	12PCH4601	SHEPHERD		5
			Total Minimum Credits	**100**

Sem: I ***Hours: 6***

Code:12PCH1101 ***Credits: 5***

ORGANIC CHEMISTRY - I

Objectives

- To learn the concept of bonding, structure and reactivity of organic molecules.
- To learn the kinetic and non-kinetic methods of determining organic reaction mechanism.

Unit I: Structure and Basic Stereochemistry

Hybridization with reference to carbon compounds-Shapes of simple organic molecules-bond angle and bond length in organic molecules. Electronegativity of atoms and groups. Dipole moments of molecules-Applications of dipole moment to study the properties of organic molecules. Polarity of solvents. Hydrogen bonding-Inter and Intramolecular hydrogen bonding.

Electronic Effects-Inductive, resonance and hyperconjucative effects and their influence-rules of resonance. Tautomerism. Steric effects and strengths of acids and bases.

Introduction to Stereochemistry-principles of symmetry-concept of chirality. Molecular symmetry and chirality. Newmann, Sawhorse, Fischer and Wedge representations and their interconversions. Types of molecules exhibiting optical activity. Configurational nomenclatures of acyclic and cyclic molecules: *cis-trans* and *E,Z* - and *D*, *L*; *R*, *S*; erythro and threo; *syn* and *anti*; *endo* and *exo*.

Unit II: Aromaticity

Aromatic character - Huckel's rule and applications-Craig's rule and applications - Consequences of aromaticity - non-altemation in bond length - Resonace energy from heat of hydrogenation, heat of combustion and Huckel's MO calculation. Deshielding effect (NMR) in aromatic compounds - magnetic susceptibility exaltations - Alternant and non-alternant hydrocarbons-antiaromtic compounds-paratropic compounds. Aromatic characterization of azulenes, tropones and annulenes.

Unit III: Reactive Intermediates

Generation, structure, stability and reactions of Carbocations (classical and nonclassical), carbanions, carbenes, nitrenes and free-radicals.

Free - radical substitution reactions - Mechanisms in aliphatic and aromatic substrates Neighbouring group assistance - Orientation and reactivity - selected reactions Hunsdieker, Kolbe, Meerwein arylation, and Hofrnann - Loffier - Fretag.

UNIT IV: Methods of Determining Reaction Mechanism

Thermodynamic and Kinetic controlled reactions.

Non-kinetic methods - Product analysis and its importance - Intermediates and Transition states - Trapping, testing and detection of intermediates - Cross over experiments. Isotopic labeling - stereochemical studies.

Kinetic methods - Order - rate and rate constants - Energy of activation-entropy of activation - Influence of solvents, ionic strength, and salt and isotopic effects on the rate of the reaction.

Correlation analysis - Linear free energy relationships - Hammett equation-singnificance of r and s - Applications of Hammett equation and Taft equation.

Unit V: Aromatic Electrophilic and Nucleophilic Substitutions

Aromatic Electrophilic substitution - Arenium ion mechanism - Reactivity - Selected reactions - Nitration - Nitrosation - Sulphonation - Halogenation - Friedel Craft's reaction, Gattermann reaction - Vilsmeir Haack reaction - Gattermann Koch reaction - Reimer Tiemann reaction-Jacobsen reacation - Bischler Napieralski reaction - Pechman reaction - Houben - Hoesch reaction.

Aromatic nucleophilic substitution - SNAr mechanism- SN1 (Aromatic) mechanism with evidences - Benzyne mechanism - Effect of substrate structure, leaving group, attacking nucleophile and solvent. Selected reactions - Von Richter, Sommelet-Hauser and Smiles rearrangements.

REFERENCES

1. Cahn RS and Derner OC, *Introduction to Chemical Nomenclature,* Butterworth, London (1968).
2. March J, *Advanced Organic Chemistry,* Fourth Edition, John-Wiley and Sons, New York (1992).
3. Sykes P, *Guide Book to Mechanism in Organic Chemistry,* Sixth Edition, ELBS with Longmann (1997).
4. Eliel E L, *Stereochemistry of Carbon Compounds,* Tata-McGraw Hill Publishing Company, New Delhi (1998).
5. Nasipuri D, *Stereochemistry of Carbon Compounds,* Second Edition, New-Age International Publishers, New Delhi (1996).

Sem: I ***Hours: 6***

Code:12PCH1102 ***Credits: 5***

INORGANIC CHEMISTRY - I

Objectives

- To understand the chemistry of transition and non-transition elements.
- To know the fundamentals and applications of nuclear chemistry.

Unit I: Transition Elements

Transition elements - General characteristics - atomic, ionic size - variation along the period and group - variable valency, colour, magnetic properties, non-stoichiometry, catalytic property and complexing tendency - Stabilization of unusual oxidation states.

Unit II: Inner Transition Elements

Inner transition elements - position in the periodic table – electronic configuration, oxidation states, solubility, colour and spectra, magnetic properties. Separation of lanthanides - lanthanide contraction: Cause and consequences - Gd break, shift reagents - Extraction of Th and U. Comparison of actinides and lanthanides.

Unit III: Selected Compounds of *d*-block elements and fundamentals of nuclear chemistry

Selected Compounds of d- block elements (Synthesis and Structure only) Chromium(II) acetate, Manganese(III) acetate, Manganese(III) oxalate, $Re_2Cl_8^{2-}$, $Nb_6Cl_{12}^{2+}$, $Mo_6Br_8^{4+}$, Prussian Blue, Turnbull's Blue, $[Ni(dmg)_2]$, [Zn(edta)], Zinc acetate.

Fundamentals of Nuclear Chemistry The nucleus - subatomic particles and their properties - nuclear binding energy -nuclear structure - Liquid drop model and nuclear shell model - n/p ratio - nuclear forces - Modes of radioactive decay - alpha, beta and gamma decay - orbital electron capture - nuclear isomerism-internal conversion.

Unit IV Instrumental Techniques in Nuclear Chemistry

Nuclear reactions - Q value, Coloumb barrier, nuclear cross section, threshold energy and excitation function-Different types of nuclear reactions with accelerated particles. Projectile capture and particles emission, spallation, fragmentation, scattering (elastic and inelastic), fission, fusion- proportional counter, Geiger-Muller counter, scintillation counter and Cherankov counter. Accelerators-linear, cyclotron, synchrotron, betatron and bevatron

Unit V Applications of Fission, Fusion and Trace Elements

Characteristics of fission reactions - product distribution, theories of fission - fissile and fertile isotopes - nuclear fusion and stellar energy, synthetic elements - Nuclear wastes-nuclear reprocessing-radiation hazards and prevention. Applications of isotopes-neutron activation analysis - isotopic dilution analysis - Uses of tracers in structural and mechanistic studies, agriculture, medicine and industry - Dating of objects - hot atom chemistry-Atomic Power Projects in India.

REFERENCES

1. Lee J D. *Concise Inorganic Chemistry,* Sixth Edition, ELBS, London, 1998.
2. Huheey J E, Keiter E A, Keiter R L and Medhi O K. *Inorganic Chemistry: Principles of Structure and Reactivity,* Fourth Edition, Pearson Education, New Delhi, 2006.
3. Cotton F A and Wilkinson G, *Advanced Inorganic Chemistry,* Third Edition, John- Wiley and Sons, New York, 1988.
4. Friedlander G, Macias E S, Kennedy J W and Miller J M, *Nuclear and Radiochemistry* (Third Edition) John Wiley and Sons Inc., London 1981.
5. Glasstone S. *Source book on Atomic energy*, Affiliated East West Press, Pvt. Ltd. New Delhi, 1967.
6. Arniker H J, *Essentials of Nuclear chemistry,* New Age International Publishers, New Delhi, 2005.

Sem: I ***Hours: 6***

Code: 12PCH1103 ***Credits: 5***

PHYSICAL CHEMISTRY - I

Objectives

- To study the fundamentals and applications of classical mechanics and quantum chemistry.
- To learn the fundamentals and applications of statistical thermodynamicsa.

Unit I: Classical Mechanics

Dynamic variables - definition, dimension, units and dimensional analysis - Coordinate systems - rectangular and spherical polar - Conversion of rectangular coordinates into spherical polar coordinates - volume element - symmetry of space and its relation to conservation laws - Conservation theorems - conservation of linear momentum, angular momentum and energy - Equations of motion - Newtonian, Lagrangian, Hamiltonian - Definition of classical mechanics, quantum mechanics and relativistic mechanics - Assumptions of classical mechanics. Classical wave equation - Conversion of classical wave equation into Schroedinger wave equation - Failure of Classical mechanics - Black body radiation - Photo electric effect - Heat capacity of substances-Hydrogen atom spectrum.

UNIT II: Mathematics for Quantum Chemistry

Functions - definition, classification-Linearly dependent and independent functions, odd and even functions-Inner product - normalization - orthogonality - ortho normal functions-Kronecker delta - proper function - Eigen functions - need for normalization. Operators - Linear, angular momentum, energy operators-Linear and non-linear operators. Hermitian operators and their properties-Proof for Hermicity of linear, angular, position and Hamiltonian operators-Commutator of operators-Commutation relation among angular momentum operators *Lx*, *Ly*, *Lz*- Vectors - vector space - Euclidean space, Hermitian space, Hilbert space.

UNIT III: Applications of Quantum Chemistry -I

Wave - particle dualism - Compton effect-Uncertainty principle and its applications - Postulates of quantum mechanics - Setting up Schroedinger wave equation and solving for particle in a 1D and 3D box, Harmonic oscillator, Rigid rotor, Hydrogen atom - Hydrogen atomic orbitals - Analytical and graphical representations -Radial probability distribution function - Orthogonality of 1s, 2s, 2p orbitals - Many electron atom - one electron orbital and one electron potential, Pauli's exclusion principle, Slater's determinant.

UNIT IV: Fundamentals of Statistical Thermodynamics

Permutations and combinations - Combinatory rule - probability theorems. Microstates, macrostates - Methods of counting microstates of distinguishable and indistinguishable particles-Heat capacity of solids - Einstein and Debye models - Maxwell - Boltzmann statistics - Phase space - Thermodynamic probability - Statistical equilibrium. Derivation of M.B. statistics - Relationship between entropy and probability - Statistical meaning of third law of thermodynamics.

UNIT V: Applications of Statistical Thermodynamics

Partition functions - Derivation of thermodynamic quantities E, S, A, H, G, K and *Cp*, *Cv* using partition function.Translational, rotational and vibrational partition functions of diatomic molecules and poly atomic molecules - Electronic partition function - Sackur - Tetrode equation - Paulis exclusion principal, Slater determinant symmetric and antisymmetric wave functions. Quantum statistics. Bose Einstein statistics - Behaviour of helium at low temperature - Fermi Dirac statistics. Electronic heat capacity of gases - Nulear spin statistics - Statistical basis of entropy of hydrogen gas, ortho and para nuclear states - Calculation of ortho-para ratio of hydrogen gas-Rotational heat capacity of molecular hydrogen, nuclear spin entropy.

TEXT BOOKS

1. Prasad R.K. *Quantum Chemistry,* I Edition, New Delhi, Wiley Eastern Ltd, (1992) - Unit 1, 2.

2. Anderson J.M. *Mathematics of Quantum Chemistry,* I Edition, Massachusetts, W.A.Benjamine Inc. (1966) - Unit 2.
3. Kuriakose. J.C. and Rajaram J.C. *Thermodynamics* Jalandar Shoban Lal Co., (1996) – Unit 4.
4. Gupta and Kumar *Classical Mechanics* – Unit 1.

REFERENCES

1. Chandra. A.K., *Introductory Quantum Chemistry,* 4th ed., Tata McGraw, Hill (1994).
2. I.N. Levine, *Quantum Chemistry,* 4th ed., Prentice hall ofInia, Pvt. Ltd (1994).
3. D.A. McQuarrie, *Quantum Chemistry,* University Science Books, (1998).
4. P.W. Atkins, *Molecular Quantum Mechanics,* Clarendon (1973).
5. Glasstone. S *Thermodynamics for chemists,* New Delhi, East West Affiliated Pvt. Ltd, (1969).
6. Gupta M.C., *Statistical Thermodynamics,* Wiley-Eastern Limited, Madras (1997).
7. Donald McQuarrie *Molecular Thermodynamics*.

Sem: I ***Hours: 4***

Code: 12PCH1104 ***Credits: 3***

ORGANIC CHEMISTRY PRACTICAL - I

Objectives

- To learn the separation of binary organic mixtures and characterize them.
- To learn some single stage preparation of organic compounds.

1. Micro Qualitative Analysis of a binary organic mixture

i. Pilot separation

ii. Bulk separation

iii. Determination of m.p/b.p

iv. Analysis

v. Derivatization

2. Semi-micro Preparation of Organic compounds (single-stage and double stage)

i. Oxidation of toluene to benzoic acid

ii. preparation of acetanilide

iii. preparation of *p*-nitroaniline from acetanilide

iv. preparation of *p*-bromoaniline from acetanilide

v. nitration of methylbenzoate

vi. *m*-nitrobenzoic acid from *m*-nitromethylbenzoate.

Sem: I ***Hours: 4***

Code: 12PCH1105 ***Credits: 3***

PHYSICAL CHEMISTRY PRACTICAL - I

Objectives

* To learn some non-electrical physical chemistry experiments.

1. Neutral salt effect - Kinetics of reaction between iodide and Persulphate - Effect of ionic strength on rate constant.
2. Polarimetry - Inversion of Cane sugar.
3. Kinetics of iodination of acetone.
4. Kinetics of hydrolysis of ester - Comparison of acid strengths.
5. Determination of Arrhenius parameters - Hydrolysis of methyl acetate by acid.
6. Partition coefficient - Study of $KI + I_2 = KI_3$
7. Phase diagram of naphthalene - *m*-dinitrobenzene system. (Simple eutectic system).
8. Heat of fusion of naphthalene.
9. Heat of solution of oxalic acid by solubility.
10. Partial molar volume of electrolytes.
11. Freundlich's Adsorption Isotherm - Adsorption of acetic acid by charcoal.
12. Phase diagram of two-component system forming a compound.

Demo experiments

1. Kinetic study under low temperature with ultra crystal circulator.
2. Phase diagram of three-component system.

Sem: I *Hours: 4*

Code:12PCH1201A *Credits:4*

CORE ELECTIVE I A - ANALYTICAL AND PHOTOCHEMISTRY

Objectives

- To study the analytical techniques, instrumentation and applications.
- To understand the principles of photochemistry.

UNIT I Error Analysis - I

Dimensional analysis - Significant figures - rounding off the values - accuracy and precision - errors - classification of errors constant errors and proportional errors - determinate errors (Systematic errors): operational (personal) errors, instrumental, reagent, methodical errors-indeterminate (random and accidental) - minimization of errors: calibration of apparatus, analysis of standard samples, running a blank determination, and independent analysis - Average, range, median, average deviation, relative average deviation and standard deviation, variance, coefficient of variation.

UNIT II Error analysis - II and Thermal Analysis

Error Analysis-II The normal error curve - testing of significance - *F*-test, *t*- test and *Q*-test - confidence limit - rejection of result - method of least squares.

Thermal analysis Thermogravimetic analysis: Principle, TGA instrumentation, Thermogram of copper sulphate pentahydrate, calcium oxalate monohydrate and silver nitrate - Factors affecting thermogram - DTA and DSC - instrumentation and Applications.

Unit III Spectrophotometric methods

Colorimetry - fundamental laws - photoelectric colorimetry - different monochromators and detectors (any one method for each) - applications - Fluorimetry and phosphorimetry - principle and applications.

Unit IV Spectroscopy and Photochemistry

Absorption and emission spectrophotometry Atomic absorption spectrometry - principle and applications. Flame photometry - principle and applications.

Photochemistry Basic laws of Photochemistry - Photo physical processes - Photo chemical processes - rate constant and life time of reactive energy states.

UNIT V Photochemical reactions

Types of photochemical reactions, photo chemistry of transition metal complexes - photo redox, substitution, light induced isomerisation, dissociation and linkage isomerisation reactions.

REFERENCES

1. Vogel A I, *A Text Book of Quantitative Inorganic Analysis*, 3rd Edn., London, Longman Group Ltd.
2. R A Day & AL Underwood, *Quantitative Analysis*, 6th Edn., PHI, *2001*.
3. Gary A Christian, *Analytical Chemistry*, 6th Edn., John Wiley & Sons Ltd., *2003*.
4. R Gopalan, P S Subramanian, K Rengarajan, *Elements of Analytical Chemistry*, 3rd Edi., Sultan Chand & Sons, New Delhi, *2003*.
5. P C Kamboj, *University Practical Chemistry*, Vishal Pub., Jalandhar, *2008.*
6. U N Dash, *Analytical Chemistry – Theory and Practice*, 2nd Edn., Sultan Chand & Sons, New Delhi, *2005*.
7. Willard and others, *Instrumental methods of analysis,* Third edition, East West Press, 1977
8. Rohatgi-Mukherjee K K, *Fundamentals of Photochemistry*, New Age International Publishers, New Delhi, 2006.

Sem: I *Hours: 4*

Code:12PCH1201B *Credits:4*

CORE ELECTIVE I B: ORGANOMETALLIC CHEMISTRY

Objectives

- To know the structure and reactivity of organometallic reagents.
- To study the applications of various orgnometallics in organic synthesisa.

UNIT I Introduction

Introduction - definition - classification, nomenclature and characteristics of organometallic compounds - classification based on hapticity, polarity of M-C bond - nomenclature of organometallics - metal atom functionality in organometallics.

UNIT II Synthesis of carbon-carbon bonds

Synthesis of C-C bonds and organometallic reagents - reactions of carbanions - introduction - alkali metal compounds - organo copper compounds - organo magnesium compounds - organo aluminium compounds - organo boron compounds - organo nickel compounds.

UNIT III Syntheis of carbon-heteroatom bonds

Synthesis of bonds linking carbon to other atoms - synthesis of C-H bonds - synthesis of bonds linking C to N, P, O, S and the halogens.

UNIT IV Synthetic applications

Organoboranes - formation of C-O bonds - formation of C-N, C-X and C-M bonds - organomercury compounds - aromatic mercuration organolithium compounds - organo thallium compounds - organo rhodium complexes.

UNIT V Biological applications

Biological applications and environmental aspects of organometallic compounds - introduction - organometallilcs in medicine, agriculture and horticulture.

References

1. Coates G E, Loff Green, Powell Kowade P. Principles of organometallic chemisty, Second Edition, ELBS with Chapmann and Hall (1988).
2. Swan N M and Black D S T C. Organometallics in organic synthesis, New York, John-Wiley (1974).
3. Mehrotra Anirudh Sigh R C. Organometallic chemistry, Wiley-Eastern Limited, New Delhi (1991).

Sem: II ***Hours: 6***

Code: 12PCH2106 ***Credits: 5***

ORGANIC CHEMISTRY - II

Objectives

- To understand the stereochemistry and its implications in molecular dynamics.
- To probe the addition, elimination, rearrangements, reductions and oxidation reaction mechanisms.

UNIT I: Stereochemistry

Stereochemistry of molecules with axial chirality-atropisomerism – biphenyls-allenes, spiranes and analogues. Helicity and chirality. Topocity and prostereoisomerism-topocity of ligands and faces-enantiotopic ligands and facesdiastereotopic ligands and faces. Racemization-methods-mechanisms of racemization through carbocations, carbanions and free-radicals.

Geometrical isomerism-*cis*, *trans* and *E*, *Z* nomenclature. Conformations of cyclic systems-conformations of mono and disubstituted three, four, five and six membered ring systems and their optical acitiviy.

Conformations of decalin. Quantitative correlation between conformation and reactivity - Winstein - Eliel equation and Curtin-Hammett principle.

Conformation, reactivity and mechanism in cyclic systems - reactions involving exocyclic atoms-saponification of esters-esterification of alcohols. Nucleophilic substitution at ring carbon atoms - SN^1 and SN^2 - formation and cleavage of epoxide rings-addition reactions to double bonds-electrophilic addition - nucleophilic addition-*cis* addition via cyclic intermediate - E_2 eliminations - pyrolytic *cis* - elimination-l,4-elimination leading to molecular fragmentation.

General reactions with reference to stereochemistry-chromic acid oxidation of cyclohexanols - Neighbouring group participation-participation of intemal nucleophile and pi-electrons of double bonds. Deamination of 2-amino cyclohexanols.

UNIT II: Aliphatic Nucleophilic and Electrophilic Substitutions

Aliphatic nucleophilic substitution SNi, SNi' and SN2' mechanisms-effect of substrate structure, leaving group, attacking nucleophile and solvent polarity-neighbouring group participation-substitution at vinylic and allylic carbons and reactivity. Ambient nucleophiles and substrates. Hydrolysis of esters-mechanisms. Selected reactionsVon-Braun, Dieckmann, Williamson.

Aliphatic electrophilic substitution SE^1 and SE^2 and SEi mechanisms - effect of substrate structure, leaving group, attacking nucleophile and solvent polarity. Selected reactions - Migration of double bonds-halogenation of aldehydes and ketones-Stork-Enamine reaction-decarboxylation of aliphatic acids - Haloform reaction.

Unit III : Addition and Elimination

Additions-Addition to carbon-carbon multiple bonds-addition mechanisms - electrophilic, nucleophilic and free-radical additions-cyclo addition - orientation and reactivity. Selected reactions - Birch reduction- Diels - Alder reaction - Hydroboration - Michael reaction.

Addition to carbon-hetero atom multiple bonds. Addition mechanisms-orientation and reactivity. Selected name reactions - Acyloin ester condensation, Aldol condensation, Benzoin condensation, Cannizaro reaction, Claisen reaction, Darzen's condensation, Knovenegal, Mannich, Stobbe and Benzoin.

Eliminations - E_1, E_2 and E_1cB mechanisms - spectrum of E_1, E_2 and E1cB mechanisms, orientation and reactivity. Bredt's rule. Selected reactions - dehydration of alcohols dehydrohalogenation - Chugeaev reaction - Hofmann exhaustive methylation - Cope elimination - Shappiro reaction. Extrusion Reactions - a few examples.

Unit IV: Oxidation and Reduction reactions

Synthetic uses of the following oxidants - SeO_2, $KMnO_4$, CrO_3, $Pb(OAc)_4$, peracids, ozone, periodate, OSO_4, DDQ, PCC, MnO_2, Jones reagent and chromyl chloride - catalytic hydrogenation and

dehydrogenation- Synthetic uses of the following reductants $NaNH_2$, Wilkinson's catalyst, LAH, $NaBH_4$, $(t\text{-}BuO)_3AlH$, $NaBH_3CN$, R_3SnH, Me_3SiCl, alkali metals, hydrazine. MPV reduction.

UNIT V: Molecular Rearrangements and Name Reactions

Classification-mechanism and applications of the following rearrangements: Baeyer - Villiger, Beckmann, Curtius, Dienone - Phenol, Favorskii, Fries, Lossen, Neber, Schmidt, Stevens, Tiffenev - Demsanov ring expansion, Bamford-Stevens reaction - Baylis-Hillman reaction - Biginelli reaction - Mukaiyama aldol reaction - Prins reaction - Mitsunobu reaction - Weinreb ketone synthesis Henry reaction - Hosomi-Sakurai reaction

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1. March J, *Advanced Organic Chemistry,* Fourth Edition, John-Wiley and Sons, New York (1992).
2. Sykes P, *Guide Book to Mechanism in Organic Chemistry,* Sixth Edition, ELBS with Longmann (1997).
3. J. Clayden, N. Greevs, S. Warren and P. Wothers, Organic Chemistry, Holt-Reinhart and Winston, New York (1959).
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6. Kalsi P S, *Stereochemistry: Conformation and Mechanism,* 4th Edition, NewAge International Publishers, New Delhi (1997).
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Sem: II *Hours: 6*

Code: 12PCH2107 *Credits: 5*

INORGANIC CHEMISTRY - II

Objectives

- To understand hybridization, bonding and structures of inorganic compounds.
- To understand the periodicity of elements and the chemistry of halogens and noble gases.

UNIT I : Ionic Bonding

Effective nuclear charge - shielding - Slater's rule - Born-Lande equation - Born Haber cycle and its applications - Radius ratio - polarization- Fajan's rule - results of polarization. Electronegativity - determination - methods of estimating charges, electronegativity equalization - Types of chemical forces- effects of chemical forces - melting and boiling points, solubility and hardness.

Unit II : Covalent Bonding

Valence bond theory – resonance – conditions of resonance – formal charge-hybridization – energetics of hybridization – Molecular orbital theory- symmetry and overlap -molecular orbitals in homonuclear diatomic molecules O_2, B_2, N_2 and C_2 – M.O. of hetero nuclear diatomic molecules; CO and HCl. MO treatment of triatomic molecules such as BeH_2. VSEPR theory – methane, ethylene, acetylene, ammonia, water, PCl_3F_2 (Bent's rule), SF_4, BrF_3, TeF_5^-, ICl_2^-, ICl_4^-, XeF_2, XeF_4, XeF_6, XeO_3, XeO_4, XeO_2F_2, $XeOF_4$, phosphorus trihalides, ammonia & NX_3 dipole moments, OF_2 and COF_2.

UNIT III : Acids and Bases

Electrode potentials and electromotive forces - applications - Acid-base concepts. Bronsted - Lowry, Lux-Flood, Usanovich, Lewis, solvent system and generalised acid base concepts - Measures of acid-base strength - steric effect and solvation effects F-strain and B-strain - Hard and soft acids and bases - acid base strength - hardness and softness - symbiosis - Theoretical basis of hardness and softness, electronegativity and hardness and softness Types of

solvents, types of reactions - autoionisation, neutralisation, precipitation, solvation, solvolysis and complex formation-*liq*. NH_3, liq. SO_2, HF and H_2SO_4 as solvents -alkali metals in *liq.* NH_3.

UNIT IV : Periodicity and the chemistry of halogens and noble gases

Periodicity

The use of *p*-orbitals in pi-bonding – *p-pi - p-pi* bonding in heavier non-metals – the use of *d* orbitals by non-metals – experimental evidence of *p-pi - d-pi* bonding – comparison of *p-pi* bonding in phosphine complexes and oxides – experimental evidences for *d*-orbital contraction and participation.

Chemistry of halogens and noble gases

Interhalogen compounds –polyhalide ions – oxyacids of heavier halogens – anomalous behaviour of fluorine – structure and reactivity of noble gas fluorides.

Unit V : Inorganic chains, rings, cages and clusters

Silicate minerals - ortho, pyro, and meta silicates - pyroxene, amphiboles - two-dimensional silicates - talc, mica and three dimensional aluminosilicates, feldspar, zeolites, ultramarine - Silicones-preparation, properties and uses - Iso and hetero-polyacids-structure of $[TeMo_6O_{24}]^{6-}$ and $[Mo_7O_{24}]^{6-}$ ions and $[PMo_{12}O_{40}]^{3-}$ ion - Polymeric sulphur nitride - borazines, phosphonitrilic compounds-trimers and tetramers - homocyclic inorganic ring systems - Concept of multi-centered bond - structure of B_2H_6, B_4H_{10}, $[B_{12}H_{12}]^{2-}$, B_6H_{10}, B_8H_{12}, $B_{10}H_{14}$, Wade's rules, *closo*, *nido*, *arachno* boranes and carboranes and "styx" code.

REFERENCES

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2. Cotton F.A. and Wilkinson G., *Advanced inorganic chemistry,* (Third Edition) London, John Wiley & Sons (1988).
3. Harry Hall Sisler.*Chemistry of Non- aqueous solvents,* Reinhold (1961).

Sem: II *Hours: 6*

Code: 12PCH2108 *Credits: 4*

PHYSICAL CHEMISTRY - II

Objectives

- To understand the symmetry molecules and its applications.
- To study the theory and applications of molecular and magnetic resonance spectrometric methods.

UNIT I: Rotational and Vibrational Spectroscopy

Basic aspects of spectroscopy - Introductory aspects - Atomic and molecular spectraCharacterization of electromagnetic radiation - Quantization of energy -Absorption and emission spectra - Region of a simple spectrum - Basic elements of spectrometer - Microwave spectroscopy-Rotation of molecules and selection rules -Diatomic molecules - Rigid and non-rigid rotator - Intensities of spectral lines - Effect of isotopic substitution-Rotational constant (B) and centrifugal distortion constant (D) - Techniques and Instrumentation - Vibration spectroscopy - Vibration of diatomic molecules - Harmonic and anharmonic oscillators - Zero point energy, dissociation energy and force constant (k). Fundamental absorption and overtones (Hot Bands; Fermi resonance) - Break down of Born - Oppenheimer approximation-Vibrations of polyatomic molecules - Fundamental vibrations and their symmetry - Influence of nuclear spin - Techniques and Instrumentation.

Unit II: Raman and Electronic Spectroscopy

Raman spectroscopy - Raman and Rayleigh scattering - Quantum and classical theories of Raman effect - Molecular polarizabiltiy - Pure rotational Raman spectra - Stokes and antistokes lines - Vibrational Raman spectra-Mutual exclusion rule - Polarised and depolarized Raman lines - Techniques and instrumentation. Electronic spectra - Electronic spectra of diatomic molecules - Franck - Condon Principle, Dissociation energy determination and dissociation products - Pre dissociation - BirgeSponer extrapolation - Fortrate Diagram. Photo electron spectroscopy – Principle - UV

and X-ray photo electron spectrometers-Molecular photoelectron spectroscopy – ESCA - Auger electron spectroscopy - Selected applications.

UNIT III: NMR , NQR and ESR spectroscopy

NMR - Hydrogen nuclei - Chemical shift and spin - spin splitting - Coupling constant (*J*). Splitting with and without chemical exchange - Interaction between spin and magnetic field - Gyromagnetic ratio - FT NMR - NQR principle and applications - ESR-Principle - Position of ESR absorptions - *g* value - Hyperfine splitting - Zero field splitting - ESR and MO theory.

UNIT IV: Rudiments of Group Theory

Principles of Group theory-Symmetry elements - symmetry operations-Properties of group - Abelian, non - Abelian and cyclic groups-Multiplication Tables - Classes - subgroups. Molecular point groups - Schoenflies symbols - Matrices for symmetry operations - Reducible and irreducible representations - Statement of Great Orthogonality theorem - Construction of character Table – Explanation of a character Table.

UNIT V: Applications of Group Theory

Applications of Group theory - Standard reduction formula relating reducible and irreducible representations - Hybridization schemes for atoms in molecules of different geometry - AB_4 tetrahedral, AB_3 triangular planar, AB linear molecules -Symmetries of vibrational modes in non-linear molecules (H_2O, NH_3 and BF_3) - Symmetries of vibrational modes in linear molecules (HCN, CO_2, C_2H_2) - Integration method - Selection rules in spectroscopy-Mutual exclusion rule - Symmetry in crystals - Hermann - Mauguin symbols. Space groups of crystals - Translational elements of symmetry - Comparision of crystal symmetry with molecular symmetry

TEXT BOOKS

1. Raman. K. V. *Group theory and its applications to chemistry,* New Delhi, TATA McGraw Hill Co, (1990) – Unit 4, 5.
2. Banwell.C.N *Molecular spectroscopy,* New Delhi, TATA McGraw Hill Co. (1997) - Unit 1, 2, 3.

REFERENCES

2. Drago.R.S *Physical methods in inorganic chemistry* New Delhi, East West Press Ltd., (1971).

3. Chang. R *Basic principles of spectroscopy* New Jersy, Englewood Cliffs (1978).

4. Straughan, B.P. and Walker, S. *Spectroscopy Vol. 2, 3,* New York, London Chapman and Hall, A Halstet Press Book, John Wely & Sons Ins. (1975).

5. G.M. Barrow, *Introduction to Molecular spectroscopy,* Tata McGraw- Hill Edition (1993).

Sem: II ***Hours: 4***

Code:10PCH2109 ***Credits: 3***

ORGANIC CHEMISTRY PRACTICAL - II

Objectives

- To learn quantitative analysis in organic chemistry.
- To learn some double stage organic preparations.
- To learn chromatographic techniques.

1. Quantitative Analysis of Organic compounds
   - i. Determination of saponification value of an oil
   - ii. Estimation of iodine value of an oil
   - iii. Estimation of phenol and aniline
   - iv. Estimation of ketone
   - v. Estimation of glucose
   - vi. Estimation of nitrogen by Kjeldhal method
   - vii. Estimation of Ascorbic acid
2. Rotary flash evaporation technique
3. Paper chromatography
4. Thin layer chromatography
5. Coloumn chromatography.

Sem: II *Hours: 4*

Code: 12PCH2110 *Credits: 3*

PHYSICAL CHEMISTRY PRACTICAL - II

Objectives

❋ To learn some conductometric and potentiometric titrationsa.

Experiments

1. Determination of Copper and Nickel by electro gravimetry.
2. Determination of standard electrode potential of Zinc and Copper.
3. Polarographic determination of Zinc ion and Cadmium ion.
4. Salting out constant – Effect of NaCl on solubility of Benzoic acid.
5. Dissociation constant of weak acid by conductivity method.
6. Determination of second-order rate constant for saponification of ethyl acetate by conductivity.
7. Conductometric acid-base titration - mixture of acids - dibasic acid.
8. Conductometric precipitation titration - iodide and chloride mixture.
9. Potentiometric precipitation titration - mixture of iodide, bromide and chloride versus silver nitrate.
10. Solubility of sparingly soluble salt by (i) Conductivty and (ii) Potentiometry.
11. Determination of equivalent conductance of a strong electrolyte at infinite dilution.
12. Potentiometric Redox titration.

Demo Experiments

- Measurement of dipole moment with dipole meter.
- Measurement of ultrasonic velocity by ultrasonic interferrometer.

SEM-II *Hours/Week - 4*
12PSK2401 *Credits - 4*

IDC-I: SOFT SKILLS

Unit 1: Effective Communication & Resume Writing 12 Hours

Effective Communication

Definition of communication, Process of Communication, Barriers of Communication, Non-verbal Communication, Johari Window, The Art of Listening, Kinesthetic, Production of Speech, Organization of Speech, Modes of delivery, Conversation Techniques, Dialogue, Good manners and Etiquettes.

Resume Writing

What is Resume? Types of Resume? Chronological, Functional and Mixed Resume, Steps in preparation of Resume.

Unit II: Group Discussion, Interview Skills & Team Building 18 hours

Group Discussion (GD)

Group Discussion Basics, GD Topics for Practice, Points for GD Topics, Case-Based and Article based Group Discussions, Points for Case Studies, and Notes on Current Issues for GD.

Interview Skills

Common interview questions, Attitude, Body Language, The mock interviews, Phone interviews, Behavioral interviews.

Team Building

Team Vs Group – synergy, Stages of Team Formation, Dabbawala-Case Study-PPT, Broken Square-Exercise, Group dynamics, Win as much as you win- Exercise, Leadership – Styles, Work ethics.

Unit III: Personality Development, Attitude & Motivation 18 hours

Personality Development

Self awareness, Assertiveness, Goal setting, Problem-solving, Conflict and Stress Management, Decision-making skills, Positive and Creative thinking, Lateral thinking, Time management.

Attitude

Concept, Significance, Factors affecting attitudes, Positive attitude, Advantages, Negative attitude, Disadvantages, Ways to develop positive attitude, Difference between Personalities having positive and negative attitude.

Motivation

Concept of motivation, Significance, Internal and external motives, Importance of self-motivation, Factors leading to demotivation.

Unit IV: Numerical Ability **8 hours**

- Average, Percentage
- Profit and Loss**,** Simple Interest, Compound Interest
- Time and Work, Pipes and Cisterns
- Time and Distance**,** Problems on Trains**,** Boats and Streams
- Calendar**,** Ratios and Proportions.

Unit- V: Test of Reasoning **8 hours**

Verbal Reasoning

- Series Completion, Analogy
- Data Sufficiency, Assertion and Reasoning
- Logical Deduction

Non-Verbal Reasoning

- Series
- Classification

References

* Aggarwal, R.S. *Quantitative Aptitude*, S.Chand & Sons.
* Aggarwal, R.S. (2010). *A Modern Approach to Verbal and Non Verbal Reasoning*. S.Chand & Co., Revised Edition.
* Alex, K. (2009). *Soft Skills*. New Delhi, S. Chand & Company Ltd.

* Covey, Stephen. (2004). *7 Habits of Highly effective people,* Free Press.

* Egan, Gerard. (1994). *The Skilled Helper* (5th Ed), Pacific Grove, Brooks/Cole.

* Khera, Shiv (2003). *You Can Win,* Macmillan Books , Revised Edition.

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* Prasad, L. M. (2000). *Organizational Behaviour, S.Chand & Sons.*

* Ravindran, G., Elango, S.P.B., Arockiam, L. (2009). *Success through Soft skills*, IFCOT Publications.

* Sankaran, K. & Kumar, M. *Group Discussion and Public Speaking*, M.I. Pub, Agra, 5th ed., Adams Media.

* Schuller, Robert. (2010). *Positive Attitudes*, Jaico Books.

* Thamburaj, Francis (2009). *Communication Soft skills*, Grace Publications.

* Trishna's (2006). *How to do well in GDs & Interviews*, Trishna Knowledge Systems.

** Yate, Martin. (2005). H*iring the Best: A Manager's Guide to Effective Interviewing and Recruiting**

Sem: III *Hours: 6*

Code: 12PCH3111 *Credits: 4*

ORGANIC CHEMISTRY - III

Objectives

- To understand spectroscopic techniques in the structural determination.
- To enumerate the various synthetic strategies of organic molecules.

UNIT I: Organic Spectroscopy - I

UV-Visible spectroscopy-basic principles of electronic transitions-correlation of electronic transitions - instrumental and sample handling techniques - differentiating geometrical and positional isomers - Woodward - Fischer rules applied to conjugated, α and β - unsaturated and aromatic systems - Factors influencing the chromophoric absorption - applications.

ORD and CD-the concept of circularly polarized light-cause of optical activity-atomic and conformational asymmetry-ORD and CD-octant rule, alpha -haloketone rule and their applications-Cotton effect and ORD curves-applications to determine the absolute configurations of monocyclic ketones and steroids.

IR spectroscopy-instrumentation and sampling techniques-types of vibrations - characteristic group frequencies and factors influencing them-quantitative studies-inter and intra molecular hydrogen bonding-conformational aspects in cyclic 1, 2- and l, 3-diols -transannular reactions in UV and IR - applications of IR.

UNIT II: Organic Spectroscopy - II

PMR spectroscopy - chemical shift - magnetic non equivalence of protons-types of coupling and coupling constants (J_1, J_2 - values etc)- Karplus equation-deuterium exchange shift reagents-correlation of chemical shift with structure-spin decoupling of exchangeable protons-applications. Fourier Transform. CMR spectroscopy - Basic principles-broad band and off-resonance decouplings applications - Brief idea about HMBC - ESR spectroscopy-applications to organic compounds.

Mass spectrometry-instrumentation-basic principles-parent, base and meta stable peaks-calculation of molecular formula-fragmentation pattern of various classes of organic compounds-applications. GC-MS.

Joint applications of UV -Visible, IR, NMR and mass spectrometric methods to structural elucidation of organic compounds.

UNIT III: Organic Synthetic Method I

Synthons and synthetic equivalents-Synthon approach-nucleophilic and electrophilic Synthons-umpolung reactions-typical examples. Retereosynthetic analysis-designing syntheses by disconnection approach. Formation of carbon-heteroatom bonds. Ring opening and ring closure reactions. Regioselective and stereoselective alkylation-cyclic ketones-cyclic enones - l,3-diketones-b-keto esters-a-halo ketones. Protecting groups- protection of hydroxyl, carboxyl, carbonyl and amino groups-illustration of protection and deprotection in syntheses.

UNIT IV: Organic Synthetic Method II

Alkylation reactions - C versus O alkylation - enamines and selective alkylation - Use of special reagents with reference to organo Cu and Cd compounds.

Uses of special reagents containing B, P and Si.

Asymmetric synthesis: nucleophilic addition to a-chiral carbonyl compounds, by chiral reagents: Chirally modified LAH and BINAL-H, by chiral auxiliaries derived from Valine, by chiral catalyst, by alkylation of carbonyl compounds, by chiral Michael addition.

Reagents in organic synthesis: DCC, *n*-Bu_3SnH, LDA, baker yeast, Me_2CuLi (Gilman's reagent)- Woodward and Prevost hydroxylations.

Olefination of carbonyl compounds: McMurry's polyolefination, Peterson synthesis, Eglinton reaction, Wittig reaction and modifications.

Phase transfer catalysis-crown ethers. Merrifield resin synthesis.

UNIT V: Photochemistry and Pericylic reactions

Photochemistry - Fndamental concepts - Joblanskii diagram-photosensitization. Photochemical reactions - photoreduction - photooxidation - photochemical rearrangements - Norrish type-I and type - II reactions - Paterno - Buchi reaction - Barton reaction - Ene reaction - Di-*pi* methane reaction - photochemistry of alkenes, dienes, carbonyl compounds and aromatic compounds-photoaddition.

Pericyclic reactions - Characteristics - types - applications of FMO and MO correlation diagram methods to electrocyclic and cycloaddition reactions - Woodward - Hoffmann rules and their applications to simple systems - cycloadditions involving hydrogen transfer - Sigmatropic reactions-Cope and Claisen rearrangements.

REFERENCES

1. March J, *Advanced Organic Chemistry;* Fourth Edition, John-Wiley and Sons, New York (1992).
2. Finar I L, *Organic Chemistry* Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997).
3. Silverstein R M and Bassler G C, *Spectrometric Identification of Organic Compounds,* Fourth Edition, John- Wiley and Sons, New York (1993).
4. Kemp W, *Organic Spectroscopy,* Third Edition, ELBS, London (1987).
5. Fleming I, *Spectroscopic Methods in Organic Chemistry,* Fourth Edition, Tata-McGraw Hill Publishing Company, New Delhi (1988).
6. Stewart Warren, Designing Organic synthesis: The Disconnection Approach, Wiley, New Delhi, (1984).

Sem: III ***Hours: 6***

Code: 12PCH3112 ***Credits:5***

INORGANIC CHEMISTRY - III

Objectives

1. To understand the theories of bonding in coordination compounds.
2. To study the kinetics and mechanisms of reactions of complex compounds.
3. To understand the spectral behaviors of complexes.

UNIT I: Theories of Coordination Chemistry

Crystal field theory - Splitting pattern of octahedral, tetrahedral, square planar, trigonal bipyramidal and square pyramidal complexes - Magnetic properties, CFSE, high spin-low spin cross over - limitations - Structural and thermodynamic effects of inner orbital splittings, Jahn - Teller effect (static, dynamic, elongation and flattening) - Ligand Field theory - Evidences for M-L overlap, spin-orbit coupling constant and Racha parameters - MO theory of Octahedral complexes(sigma and pi bonding) - MO of *Td* and square planar complexes.

UNIIT II: Carbonyl and Nitrosyl complexes

Carbonyls - bonding - terminal, double, triple bridged carbonyls - structure of carbonyls - CO stretching frequencies of carbonyl and mixed carbonyls - Nitrosyls: terminal, bridging and bent - phosphine derviatives, cyanides, and complexes of N_2 and O_2. *pi*- complexes with olefins, acetylenes, 1,3-butadienes ligands - ferrocene and benzenoid metal complexes. Non-benzenoid aromatics as ligands- fluxional molecules.

UNIT III: Reaction Kinetics in Coordination Chemistry

Inert and labile complexes - Stepwise, overall stability constants - Chelate effect - mechanisms - SN^1, SN^2, Solvent intervention, ion pair formation and SN^1CB - evidences - Acid and base hydrolysis - mechanisms - evidences, trans effect - theories and Applications - Electron transfer reactions - inner and outer sphere

mechanisms - remote and adjacent attacks - Catalysis by organometallic compounds - oxidative addition - insertion - hydrogenation (Wilkinson's catalyst) - hydroformylation - Wacker process, Fischer - Tropsch reaction, Zeigler - Natta Catalyst.

UNIT IV: Physical Methods in Coordination Chemistry -I

Types of magnetic behaviour - magnetic susceptibility measurements - Gouy method. Orbital contribution-Spin-orbit coupling and its effect on magnetic properties. Temperature independent paramagnetism (TIP) - Electronic spectra of complexes - bandwidth and intensity, Sugano Tanabe and Orgel Diagrams - charge transfer spectra-Infrared spectra of Coordination complexes - characteristic frequencies-mode of coordination and interpretation of ClO_4^-, SO_4^{2-}, CO_3^{2-}, ester, amine, amide, DMSO and urea using IR spectra.

UNIT V: Physical Methods in Coordination Chemistry -II

NMR – Applications of NMR to inorganic compounds - NMR of metal hydrides(1H NMR), metal carbonyls(^{13}C NMR), ^{19}F and ^{31}P NMR –

ESR –zero field splitting - Krammer's degeneracy - pattern for number of lines of complexes having *d*1-*d*9 systems - bis(salicylaldimine)Cu(II), Mn(II) complexes - **Mossbauer spectroscopy** - quadrupole interactions - magnetic interactions - $FeSO_4$, $FeCl_3$, ferro- and ferricyanide, nitroprusside, $Fe_3(CO)_{12}$, I_2 Br_2Cl_4.

REFERENCES

1. Cotton F.A. and Wilkinson G, *Advanced inorganic chemistry,* (Third Edition) London, John Wiley & Sons (1988).
2. Lewis J and Wilkins R G, *Modern Coordination Chemistry,* Interscience Publishers, Inc., New York (1960).
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4. Basalo F and Pearson R G, *Mechanisms of Inorganic Reactions,* John-Wiley and Sons Inc., New York (1960).

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6. Straughn B P; Walker S*; Spectroscopy* Vol., London, Chapman & Hall, 1976.
7. Ebsworth EAV; *Structural Methods in Inorganic Chemistry*, 3rd Ed, Great Britain, ELBS, 1987.
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9. Gibbs T C; *Principles of Massbauer Specroscopy*, London, Chapman & Hall, 1976.

Sem: III *Hours: 6*

Code: 12PCH3113 *Credits: 5*

PHYSICAL CHEMISTRY - III

Objectives

- To understand the theories of kinetics of reactions and catalysis.
- To understand the theories of kinetics of electrochemical reactions.

Unit I: Theories of reaction rate

Theories of reaction rates and reaction mechanism - Arrhenius equation - Potential energy surfaces and reaction coordinates - Collision theory - ARRT (thermodynamic and statistical treatments) - Application of ARRT to unimolecular, bimolecular and termolecular ractions - Kinetic isotope effect, isokinetic relation and temperature - Theories of unimolecular ractions - Lindemann and RRK - Principle of microscopic reversibility and detailed balancing.

Unit II: Application of ARRT to solution kinetics

Application of ARRT to solution kinetics - Factors affecting reaction rate in solution. Internal pressure - Solvent dielectric constant - Ionic strength - Hydrostatic pressure - Ion-dipole and dipole-dipole reactions - vant Hoff equation and volume of activation - Acid - base catalysis - vant Hoff and Arrhenius intermediates - Mechanism - protolytic and prototropic catalysis laws - Acidity functions - Hammett - Zucker hypothesis - Catalysis in biological systems. Michaelis - Menten equation – Lineweaver - Burk and Eadie - Hofstee plots - Influence of substrate concentration, pH, temperature on rate - Influence of substituents on reaction rates - Hammett and Taft equations - Linear free energy relations.

Unit III: Surface Chemistry, Heterogeneous Catalysis and Radiation Chemistry

Surface phenomenon - Physical and chemical adsorption - Adsorption and free energy relations at interface - Langmuir adsorption isotherm - Gibbs adsorption isotherm-BET isotherm -

Measurement of surface area - Heterogeneous catalysis - Mechanism – Langmuir - Hinshelwood Mechanism – Langmuir - Rideal bimolecular mechanism - Role of surface in catalysis - Radiation chemistry - Sources of high energy radiations - Interaction of high energy radiations with matter - Detection of radiations – Dosimeters - Primary and secondary processes. Radiolysis of water - Hydrated electron - G-value.

Unit IV: Debye - Huckel Theory and its Applications

Debye Huckel theory - Radius of ionic atmosphere - Calculations of thickness of ionic atmosphere - Evidences in favor of ionic atmosphere - Asymmetry effect - Electrophoretic effect. DebyeFalkenhagen effect - Wien effect - Debye - Huckel Onsager equation - Modification and verification of the equation - Debye - Huckel limiting law - Modification and verification - Finite ion size model - Huckel -Bronsted equation - Calculation of activity coefficient - Determination of ion size parameter - solubility - solubility product of sparingly soluble salt - common ion effect - neutral salt effect and solubility - determination of solubility and solubility product.

Unit V: Electrode Kinetics

Theories of electrical double layer - Electric double layer at the electrode - electrolyte interface - Helmholtz model of double layer - Law of electro neutrality - Gouy - Chapman diffused charged model - Adsorption theory of double layer - Stern's model, triple-layer theory. Electro capillary phenomenon - Electro capillary curves for solutions containing anions, cations and molecular substances - Electro capillary maximum - Lipmann equations and Lipmann potential - Experimental measurement and calculation of Lipmann potential - Capillary electrometer and contact angle method - Electro kinetic phenomena – Classification - Electro osmosis and electrophoresis - Streaming potential and sedimentation potential - Kinetics of electrode process - Equilibrium and non-equilibrium process -Concentration and activation polarization - Theory of electrochemical over potential - Derivation and verification of the

equations – Butler - Volmer equation - Tafel equation - Hydrogen over potential - Mechanism of hydrogen evolution reactions - pH and metal deposition - Application of hydrogen over potential.

TEXT BOOKS

1. Laidler. K.J *Chemical Kinetics* III edition, New Delhi TATA McGraw Hill Co., (1984).
2. Kuriacose and Rajaram, *Kinetics and Mechanism of chemical transformation,* Macmillan &Co., (1993).
3. G. Huges, *Radation Chemistry,* Oxford series (1973).
4. L. Antorpov, *Theoritical Electrochemistry,* Mirpublishers, Mascow.
5. Bockris J O'M and Reddy A K N, *Modern Electrochemistry Vol 1 & 2,* Second Edition, Plenum Press, New York (1998).
6. Glasstone.S *An Introduction to electrochemistry,* New Delhi, East West Press Pvt. Ltd. (1956).

Sem: III *Hours: 4*

Code:12PCH3114 *Credits: 3*

INORGANIC CHEMISTRY PRACTICAL - I

Objectives

- To learn the qualitative analysis of common metals and rare metals.
- To learn colorimetric analysis.
- To learn to prepare inorganic complexes.

Experiments

1. Systematic qualitative analysis of mixtures containing 4 cations of which 2 are rare.
2. Colorimetric estimation of iron, copper, nickel and manganese.
3. At least three standard inorganic preparations from literature.

Sem: III *Hours: 4*

12PCH3202A *Credits:4*

CORE ELECTIVE - IIA : NATURAL PRODUCTS

Objectives

- To learn the chemistry of carbohydrates, proteins, nucleic acids and hormones.
- To understand the structure and functions of some natural products from plants.

UNIT I: Carbohydrates

Carbohydrates - ring structures - Determination of configuration of monosaccharidesconfiguration of C_1 in glucose-Hudson's rule-methods of determining ring size. Conformational analysis of D(+)- fructose, sucrose, maltose, lactose and cellobiose. Structural difference between starch and cellulose.

UNIT II: Proteins & Nucleic acids

Proteins - Amino acid synthesis (Strecker synthesis and Gabriel synthesis) - peptide synthesis (Merrifield resin synthesis) - End group analysis - structure of proteins - primary, secondary, tertiary and quaternary.

Nucleic acids

Structures and numbering of Purines (Uric acid, Cytosine, Adenine, Guanine) & Pyrimidines (Uracil, thymine & Cytosine). Nucleic acids - chemistry of nucleic acids- structure and biological implications of DNA and RNA *(m*-RNA, *t*-RNA and *r*-RNA)

UNIT III: Hormones

Hormones-introduction-chemical nature. Prostaglandins-structure and formation (structural elucidation not required). Structural elucidation of cholesterol (synthesis not required). Sex hormones-structural synthesis and properties of oestrone, equilinin, androsterone, testosterone (elucidation not required).

UNIT IV: Alkaloids, Terpenoids, Antibiotics and Vitamins

Alkaloids:Introduction-extraction-classification-medicinal values-structural elucidation of papaverine.

Terpenoids: Introduction - extraction - classification - structural elucidation of zingiberene **Antibiotics**: structure - Activity - structural elucidation of chloramphenicol - structure and functions of penicillin, streptomycin and terramycin.

Vitamins: structure and functions of Vitamins A_1, A_2, B, B_{12}, C, E and K (structural elucidations not required).

Unit V: Heterocyclics

Preparation, physical properties and reactions of 5-membered heterocyclic compounds containing one (pyrrole, furan, thiophene and indole) and six membered heterocyclics (pyridine, Quinoline and isoquinoline). Only the structures and numbering of diazins (pyrazine, pyrimidine and pyrazine), azines (oxazine and azepine).

References

1. Finar I L, *Organic Chemistry* Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997).
2. Jayashree Gosh, Textbook of Pharmaceutical chemistry, S.Chand & chand publications, New Delhi, (1997).

Sem: III *Hours: 4*

Code:12PCH3202B *Credits: 4*

CORE ELECTIVE II-B: PHARMACEUTICAL CHEMSITRY

Objectives

- To learn the chemistry of drugs and drug action.
- To know the common diseases and their treatment.

Unit-I Introduction to Chemistry of Drugs

Drugs - definition - sources - study of drugs - classification (Biological chemical, commercial and utility) - Nomenclature of drugs - Biotransformation - Drug design - factors affecting the stability of drugs - Encapsulation - drug delivery systems and sustained release of drugs.

Unit-II Pharmaceutical Aids

Preservatives - Antioxidants - Sequestering agents - Emulsifiers - Colorants - m Flavoring agents - Sweeteners - Stabilizers - suspending agents - Ointment bases - Solvents.

Unit-III Common Diseases and Treatment

Insect borne diseases - Treatment using drugs – Air borne diseases - Treatment using drugs - water borne diseases - Treatment using drugs - Digestive disorders - treatment - diseases of respiratory system - treatment - diseases of nervous system - treatment - Other common diseases - treatment.

Unit-IV Pathogenicidal Drugs

Antibiotics - Classification - Chloramphanicol - penicillin - streptomycin - Tetracycline - Macrolides - Erythromycin - Rifamycin - Antiseptics and disinfectants - Phenols Halogen compounds - Analgesics - Antipyretics - Anti - inflammatory agents - Sulpha drugs.

Unit-V Bio Regulatory Drugs

Cardiovascular drugs - Cardiac glycosides - anti arrhythmic drugs - antihypertensive agents - antianginal agents. Diabetes and

Hypoglycaemic drugs - two types of diabetes - Insipidus and mellitus - Control of diabetes - Insulin - Hypoglycaemic agents. Anticonvulsants - Cancer and antineoplastic drugs - Common causes - antimetabolites.

Reference

Jayashree Gosh, Textbook of Pharmaceutical chemistry, S.Chand & chand publications, New Delhi, (1997).

Semester III ***Hours: 4***

Code:12PCH3402 ***Credits: 4***

IDC-II: HEALTH CHEMISTRY

Objectives

- To know the essentials of health, drugs.
- To learn the functions of enzymes, hormones and body fluids.
- To know common diseases and their treatment.

UNIT I : Health

Definition: Food, Food Pyramid - Health-Hygiene- mal-, under- and over- nutrition, their causes and remedies, sanitation, Carbohydrates - Classification, Biological functions, Protein- Classification, Biological functions, vitamins - Classification, Biological functions

UNIT II : Drugs

Drugs - Types of drugs-depressant, anticonvulsant, narcotics, antipyretics, antibiotics, antiseptics, analgesics, muscle relaxants and cardiovascular and vasodepressants, Steroids

Unit III : Body fluids

Blood volume, groups, coagulation, blood pressure, anemia, blood sugar, hemoglobin- chemistry of respiration-urine-electrolyte balance.

Unit IV : Enzymes, Hormones, Digestion

Types of enzymes and enzyme action, Characters of hormones - action, examples of essential hormones - digestion in mouth, stomach, intestine and pancreas - mineral metabolism

Unit V : Common Diseases

Toxicants in food- cancer-types and causes- common diseases - Jaundice, vomiting, fever, rickets, scurvy, beriberi, pellagra, night blindness, ulcer, gout, goiter, diabetes, anemia and their causes.

References

1. Deb A C, *Fundamentals of Biochemistry*, New Central Book Agency, Calcutta, 1994.
2. Satake M and Mido Y, *Chemistry for Health Science*, Discovery Publishing House, New Delhi, 2003.
3. Jayashree Ghosh, A *Text book of Pharmaceutical Chemistry*, S. Chand and Co. Ltd., 1999.
4. Ashutosh Kar, Medicinal Chemistry, Wiley Easterns Limited, New Delhi, 1993.
5. Alex V Ramani, Food Chemistry, MJP Publishers, Chennai, 2009.

Sem: IV *Hours: 4*

Code: 12PCH4115 *Credits: 3*

ORGANIC CHEMISTRY - IV

Objectives

- To learn the basics of green chemistry and organometallic reagents in synthesis.
- To understand the principles of electroorganic reactions.

Unit I: Green Chemistry and Basics of Organometallics

Green Chemistry: The 12 principles, atom economy for addition, elimination, substitution reactions ant its calculation, green starting materials, green reagents, green catalysts and green reactions

Basics of Organometallics: Introduction-Formation of organometallics (Mg, Li) - Oxidative insertion of Mg and Li into alkyl halides, deprotonation of alkyne, ortholithiation of functionalized benzene rings, halogen metal exchange, transmetallation - Applications

Unit II: Organometallics in Organic Synthesis

Formation of C-C bonds: **Palladium based reactions**: Heck reaction, Suzuki coupling, Stille coupling, Sonogashira reaction, Fukuyama Coupling**. Nickel based reaction:** Negishi Coupling**,** Kumada Coupling. **Copper based reaction**: Chan-Lam Coupling. Hiyama coupling - Corey - Fuchs Reaction, Me_2CuLi (Gillman's reagent).

Unit III: Stereoselective Reactions in Cyclic Compounds

Reactions on small rings - stereochemical control in six membered rings - conformational control in the formation of six membered rings - stereochemistry of bicyclic compounds -fused bicyclic compounds - spirocyclic compounds - reactions with cyclic intermediates or cyclic transition states - stereoselective reactions of acyclic alkene compounds.

UNIT IV: Electro Organic Chemistry

Electroorganic Reactions - Basic requirements for conducting electro-organic syntheses - Effects of variables-Reduction of carbonyl,

nitro and carbon-halogen bonds-oxidation of unsaturated compounds-electro initiated polymerization.

Unit V: Organic Reactions - A Review

Routine functional group transformations and inter conversions of simple functionalities. Problems involving prediction of products of organic reactions - Problems in proposing mechanisms of organic reactions - Assigning reagents for organic reactions-introducing and inter converting functional groups in organic compounds - Problems involving transformation of organic compounds.

References

1. March J, *Advanced Organic Chemistry;* Fourth Edition, John-Wiley and Sons, New York (1992).
2. Paula yurkanis Bruice, *Organic Chemistry, Fourth Edition*.
3. Finar I L, *Organic Chemistry* Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997).
4. Jonathan **Clayden,** Nick **Greevs,** Stuart **Warren and** Peter **Wothers** , *Organic chemistry.*
5. Fifield F W and Kealy D, *Principles and Practice of Analytical Chemistry*, 5th Edition, Blackwell Science Ltd., London, 2000
6. Paul T Anastas, *Text Book on Green Chemistry*, OUP, 2006.
7. Mendham J, Denney R C, Barnes J D and Thomas M J K, *Vogel's Textbook of Quantitative Chemical Analysis*, Sixth Edition, Pearson Education, New Delhi, 2000.

Sem:IV ***Hours: 4***

Code:12PCH4116 ***Credits:3***

INORGANIC CHEMISTRY - IV

Objectives

- To understand the various structures of solid inorganic molecules.
- To understand the chemistry of crystalline defects and their effects.
- To study the chemistry of biological processes.

UNIT I : Solid State –I

Elements of crystallography - space lattices-unit cell-crystal systems - X-ray diffraction Bragg's method- Rotating crystal method and powder methods- indexing of crystal planes - Structure of typical lattices such as sodium chloride, cesium chloride. Zinc blende, wurtzite, rutile, fluorite, antifluorite, pervoskite and ReO_3 structure.

UNIT II : Solid State –II

Spinels and anti-spinels - Applications of CFT - covalent crystals diamond and graphite - Crystal Structure and properties. Types of solids, stoichiometric defects - point, line and plane defects - colour centers - non-stoichiometric defects - n, p semiconductors - structure of solids- free electron and band theory of solids. Electrical conductivity and superconductivity - high temperature superconductors.

UNIT III : Solid State -III

Structure of alloys, intermetallic compounds- interstitial compounds, clathrates - metal cluster compounds-crystal growth methods from chemical reaction, liquid solution, diffusion, fused salt electrolysis and by chemical vapour transport.

Bioinorganic chemistry - I

Essential, non-essential and toxic elements, Ionophores - Ion transport mechanism in cell membrane - Na and K pumps.

Unit IV : Bio-inorganic Chemistry –II

Synthetic oxygen carriers - Structure and characteristic features of haemoglobin and Myoglobin - Cytochromes - vitamin B_{12}, Blue copper proteins and cis-platin Ferredoxins.

UNIT V : Bio-inorganic Chemistry-III

Chlorophyll - Mechanism and role of Mn in Photosynthesis - Metal ion interaction with nucleic acids - metal ions involvement on replication, transcription and translation - Nitrogen Fixation - *in vivo* and *in vitro* - transition metal ions in biology.

REFERENCES

1. Azaroff, *Introduction to solids,* Tata McGraw Hill Publishing Co., New Delhi, 1994.
2. Evans R C, *Crystal Chemistry,* Cambridge University Press, London, 1964.
3. Addison W E, *Structural Principles of inorganic compounds,* Longmans, London, 1961.
4. Lipson, *Determination of Crystal Structures,* (Volume 3) Bell Publications, New York, 1953.
5. Rao C N R, *Solid State Chemistry,* Marcel & Dekker Inc., New York, 1974.
6. Rao, C N R, *Phase Transitions in Solids,* McGraw-Hill Co., New York, 1978.
7. Keer H V, *Principles of Solid State,* Wiley Eastern Ltd, New Delhi, 1993.
8. Arora *Solid State Chemistry,* Anmol Publications New Delhi, 1980.
9. Eichron G L, *Inorganic Biochemistry,* Elsevier publications, New York, 1975.
10. S.J. Lipard and J.M. Berg, *Principles of Bioinorganic chemistry,* Panima Publishing Corporation, 2005.
11. W. Kaim and B. Schwederski, *Bioinorganic chemistry: inorganic elements in the chemistry of life*, John willy, 1994.
12. K. Hussain Reddy, *Bioinorganic chemistry*, New Age international publishers, 2007.

Sem: IV *Hours: 4*

Code: 12PCH4117 *Credits: 3*

PHYSICAL CHEMISTRY - IV

Objectives

- To understand the electroanalytical techniques, instrumentation and applications.
- To understand the concepts and applications of quantum chemistry and polymer chemistry.

Unit I: Electro analytical Techniques -I

Polarography - Experimental set up - Advantages of dropping mercury electrode Supporting electrolyte - Maxima suppressor - Residual current - Migration current - Diffusion current - Polarogram, half wave potential - Ilkovic equation (derivation is not required) - Outline of applications (Polarogram of Zn^{2+} and Cd^{2+}) - Cyclic voltametry, Principle, Experimental set up - Cyclic voltammogram of Fe^{2+} in H_2SO_4 - Anodic peak current - Cathodic peak current - Electrochemically reversible couple - Cathodic peak potential - Electrochemically irreversible couple -Outline of applications.

UNIT II: Electro analytical Techniques II

Amperometry - Principle of amperometric titration - Different types of current - voltage curves - Amperometric titration between Pb^{2+} and $K_2Cr_2O_7$ Electrogravimetry, Principle, Experimental set up - Physical characteristics of metal deposits Separation of Cu & Ni - Coulometry, Principle, Experimental set up - Controlled potential coulometric analysis and application - Experimental set up for constant current Coulometry - Coulometric titration of Fe(II) with Cerium(III).

UNIT III: Applications of Quantum Chemistry -II

Approximation methods - Need for approximation - Perturbation Theory - Time independent Perturbation (First order only) - Application of Perturbation theory to particle in one dimensional box, anharmonic oscillator and helium atom - Principle

of variation and its proof - Variation methods and its applications to hydrogen and helium atoms.

UNIT IV : Applications of Quantum Chemistry -III

The Born - Oppenheimer approximation - MO & VB theories as applied to hydrogen molecular ion (H^{2+}) and hydrogen molecule - coulomb integral an exchange integral and an overlap integral. Construction of sp, sp^2 and sp^3 hybrid orbitals - Huckel molecular orbital theory - principles and applications to ethylene, butadiene and benzene. Huckel calculation of pi- electron energies.

UNIT V: Polymer Chemistry

Kinetics of polymerization - Free radical polymerization - Cationic polymerization - Anionic polymerization - Emulsion polymerization - Number average molecular weight of polymers - Molecular weight by Cryoscopy, ebullioscopy, Osmotic pressure method - Average molecular weight determination - Light scattering method - Using ultra centrifugation by sedimentation equipment - Sedimentation velocity - Differential scanning colorimetry - Differential thermal analysis - Thermo gravimetric analysis - Models of viscoelastic behaviour - Hooke model -Newton model - Voigt model - Burger Maxwell model - Kelvin - Voigt model -Glass transition temperature - Measurement of Tg - molecular interpretation of Tg.

TEXT BOOKS

1. Vogel A.I, *Text book of Quantitative Inorganic analysis* ELBS, 1978 – Unit 1, 2.
2. Donald A McQuarrie, *Quantum chemistry*, Indian Edition, Viva Books Private Limited (2005)- Unit 3, 4.
3. Gowarikar VR., et aI., *Polymer Science,* Wiley Eastern Ltd, 1986 – Unit 5.
4. Billmeyer, "*Text book of Polymer Science*" John-Wiley and Sons, 1996 – Unit 5.
5. Journal of Chemical Education, 1983, 60, 252-308 - Unit 1.

REFERENCES

1. Noel M and Vasu K.I., *Cyclic voltammetry and the Frontiers of Electrochemistry,* Oxford and IBH, 1990.
2. Journal of Chemical Education, 1983, 60, 687-706.
3. Kissinger, P.T. and Heinman, Laboratory Techniques in Electroanalytical Chemistry, Editors, Marcel Dekker, Inc., New York, 1984.
4. Willard, Merit, Dean and settle "*Instrumental Methods of Analysis*" CBS Publication, 1986.
7. Anatharaman R, *Fundamentals of Quantum Chemistry,* McMillan, New Delhi, 2001.
6. Prasad R.K., *Quantum Chemistry,* Wiley Eastern Ltd, New Delhi, 1992.
7. Chandra A.K., *Introduction to Quantum chemistry,* Tata-MaGrawHill, New Delhi, 1997.
8. Deshpande D.D., *Physical Chemistry of Macromolecules,* Vishal Publications, New Delhi, 1986.

Sem:IV *Hours: 4*
Code:12PCH4118 *Credits: 3*

INORGANIC CHEMISTRY PRACTICAL - II

Objectives

- To learn quantitative separation of metal ions in binary mixtures.
- To learn simple single stage preparations of some complex compounds.

1. Quantitative analysis of a mixture of iron (volumetry) and copper (gravimetry)
2. Quantitative analysis of a mixture of copper (volumetry) and nickel (gravimetry)
3. Quantitative analysis of a mixture of iron (volumetry) and zinc (gravimetry)
4. Preparation of any three complexes
5. Determination of meff of a complex by Gouy method (internal evaluation only)
6. IR interpretation of a complex to find out the mode of coordination (internal evaluation only)
7. Interpretation of electronic spectrum of a complex (internal evaluation only)

REFERENCES

1. Vogel A I, *A Text Book of Quantitative Inorganic Analysis*, 3rd Edn., London, Longman Group Ltd.

Sem:IV *Hours: 4*

Code:12PCH4203A *Credits: 4*

CORE ELECTIVE III A - APPLICATIONS OF THERMODYNAMICS AND ELECTROCHEMISTRY

Objectives

- To understand the equilibrium thermodynamics.
- To inculcate interest in solving thermodynamic problems.

UNIT I: Chemical Thermodynamics I

Partial molar properties - Need of Partial molar properties - Physical significance - Methods of determination of partial molar volume. Chemical potential - Gibbs-Duhem equation -Chemical potential of mixture of gases - Chemical potential in terms of E, H - Variation of chemical potential with temperature and pressure - Differential and integral heats of solution - Free energy of mixing and volume of mixing.

UNIT-II: Chemical Thermodynamics II

Fugacity - Definition-Methods of determination - Variation of fugacity with temperature, pressure and composition - Duhem-Margules equation - Fugacity of solids, liquids and mixture of gases - Determination of fugacity in gas mixtures (Lewis-Randall Rule) - Determination of fugacity in liquid mixtures.

UNIT III: Chemical Thermodynamics III

Activity and activity coefficients - Definition - Standard state, reference state, choice of standard state for gases, liquids and solids, liquid solvent and solute - Determination of activity coefficient of non electrolyte - Mean ionic activity - Determination of activity coefficient of electrolytes by freezing points.

UNIT IV: Numerical Problems in thermodynamics

Simple Numerical calculations on I law and II law of thermodynamics - Reversible isothermal process of ideal and real gases - Irreversible isothermal process of ideal and real gases- Reversible adiabatic process of ideal and real gases - Irreversible adiabatic process of ideal and real gases - Joule Thomson effect

UNIT V: Electrochemistry and its applications-II

EMF and thermodynamic quantities - Nearnst equation - Gibbs Helmholtz relation and EMF - Reversible electrodes - Types - electrode potentials - single electrode potentials - electrochemical series - chemical cells - concentration cells with and without transport - Liquid Junction Potentials - Application of EMF measurement - Activity coefficients and solubility determination-Storage and fuel cells.

References

1. Kuriakose. J.C. and Rajaram J.C. *Thermodynamics* Jalandar Shoban Lal Co., (1996) - Unit 1, 2, 3 and 4.
2. Antropov. L. Theoretical electrochemistry, Moscow, Mirpublishers (1972).
3. Bockris. J.O.M. and Reddy, A.K.N. Modern electrochemistry volumes I and II. New York, Plenum Press (1970).

Sem:IV *Hours: 4*

Code: 12PCH4203B *Credits: 4*

CORE ELECTIVE III B - THERMODYNAMICS

Objectives

- To understand the non-equilibrium thermodynamics.
- To study the experimental techniques to measure the thermodynamic quantities.

UNIT-I

3rd law of thermodynamics - Thermochemistry - Kirchoff's equation.

UNIT-II: Near Equilibrium Thermodynamics- I

Introduction to non equilibrium thermodynamics - Methods of study of non-equilibrium thermodynamics - Mass conversion, de-Donder equation - Energy conservation - Entropy production in systems involving heat transfer - Entropy production in chemical reactions -Affinity and equilibrium constant.

Unit III: Near Equilibrium thermodynamics -II

Affinity and Gibbs free energy - Affinity and rate derivations - Coupled and non coupled reaction systems - Entropy production and entropy flow in open system - Onsager Theory - Phenomenological relations - an introduction - Characteristics of direct and cross coefficients - Rate expression using Onsager equation - Kinetic approach - Thermodynamic approach - Derivation of On - sager reciprocity relation using a cyclic coupled reaction (Proof of $L_{12} = L_{21}$)

UNIT IV: Near Equilibrium Thermodynamics -III

Linear law - Condition for coupled and non-coupled reactions with reference to cross coefficients - Decomposition of cyclohexane and linear law - Non-coupled reaction -Isomerization of xylene - Coupled reaction - Reaction taking place in liver - Experimental verification of Onsager's reciprocity relation – Thermoelectricity - Seebeck effect - Peltier effect - Electro kinetic effect – Thermo

molecular pressure difference - $L_{12} = L_{21}$ by transference number method - Irreversible thermodynamics and biological systems.

UNIT V: Experimental Methods in Thermodynamics

Experimental methods used in thermodynamics - Determination of ΔH, ΔS, ΔG - determination of heat of mixing and volume of mixing - Adiabatic compressibility (ultrasonic interferometer) - Bomb Calorimeter - Vapour pressure by isoteniscope method.

TEXT BOOK

Kuriakose J.C. and Rajaram J.C. *Thermodynamics* Jalandar Shoban Lal Co., (1996)- Unit 1, 2, 3, 4, 5.

REFERENCES

1. Glasstone. S *Thermodynamics for chemists,* New Delhi, East West Affiliated Pvt. Ltd., (1969).
2. M.C. Gupta, *Thermodynamics*, Wiley - Eastern Limited, Madras (1997).
3. Lewis and Randall *Thermodynamics*.
4. Puri and Sharma, *Principles of Physical Chemistry*, Vishal publishing & Co.

INTER DEPARTMENTAL COURSE – IDC

BIOCHEMISTRY

12PSK2401 SOFT SKILLS

12PBI3402 FIRST AID MANAGEMENT

BIOTECHNOLOGY

12PSK2401 SOFT SKILLS

12PBT3402 APPLIED BIOTECHNOLOGY

BOTANY

12PSK2401 SOFT SKILLS

12PBO3402 HORTICULTURE & LANDSCAPING

CHEMISTRY

12PSK2401 SOFT SKILLS

12PCH3402 HEALTH CHEMISTRY

COMMERCE

12PSK2401 SOFT SKILLS

12PCO3402 FINANCIAL ACCOUNTING FOR MANAGERS

COMMERCE (CA)

12PSK2401 SOFT SKILLS

12PCC3402 CAREER PLANNING AND MANAGEMENT

COMPUTER APPLICATIONS

12PSK2401 SOFT SKILLS

12PCA3402 COMPUTER APPLICATIONS FOR SOCIAL SCIENCES

12PCA3403 FUNDAMENTALS OF PROGRAMMING

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HISTORY

12PSK2401 SOFT SKILLS

12PHI3402 INDIAN CONSTITUTION

HUMAN RESOURCE MANAGEMENT

12PSK2401 SOFT SKILLS

12PHR3402 FUNDAMENTALS OF HRM

INFORMATION TECHNOLOGY

12PSK2401 SOFT SKILLS

12PIT3402A FLASH

12PIT3402B WEB DESIGN

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12PMA3402 OPERATIONS RESEARCH

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12PPH3402 MODERN PHOTOGRAPHY

TAMIL

12PSK2401 நுண்வகைமைத்திறன்கள்

12PTA3402 அரசுப்பணித்தேர்வுத் தமிழ் - I