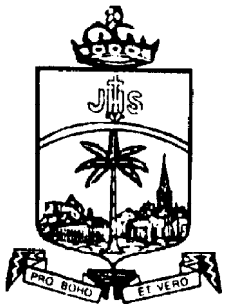
M.Sc. CHEMISTRY

SYLLABUS: 2010-2012

CHOICE BASED CREDIT SYSTEM
(CBCS)



St. JOSEPH'S COLLEGE (Autonomous)

Re-accredited with A⁺ Grade 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, Reaccredited with A+ Grade from NAAC (2006), 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	Additional
I – IV	3 – Core Electives	3	4	3 x 4	12
	2 – Inter Dept. Courses (IDC)	2	4	2 x 4	08
I – IV	SHEPHERD – Extension Activity	~	70	5	Additional

Total Minimum Credits	90
Total Additional Credits (Compulsory)	10
Other Additional Credits (Dept. Specific)	....

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

For PG courses a student must earn a minimum of 90 credits and 10 compulsory credits as mentioned in the above table. 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 Department 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 Practical, Projects, Group Discussion, Viva, Field Visit, 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 Department 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.

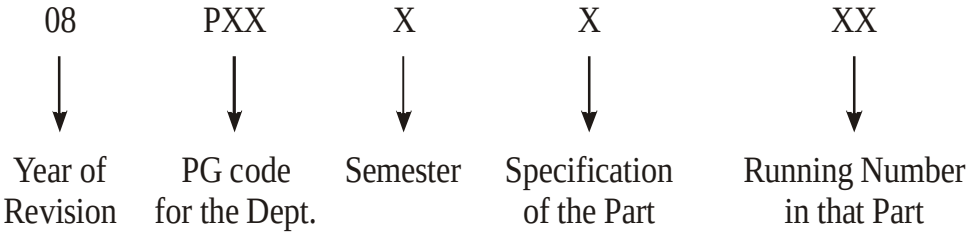
Day College (Shift-I) student may also take an IDC from SFS (Shift-II) course and vice versa

This provision enables students to earn extra credits. For the Shift – I students it is offered in their last hour and for the Shift-II

(Course) students in their first hour. 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 (compulsory)
06 – Shepherd (compulsory

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 1 hour and 30 minutes duration. The remaining 40% would comprise of any four 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.
- 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.

Question Pattern

Pattern	Mid & End Semester Test	Semester Exam
Part A : Objective	10 x 0.5 = 05	20 x 1 = 20
Part B : Either/or type	3 x 3 = 09	5 x 6 = 30
Part C : Comprehensive	(2/3)2 x 8 = 16	(5/6)5 x 10 = 50
	Total = 30	Total = 100

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 Ci is the credit earned for that course in any semester and Mi 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

The performance in Compulsory credits in Project and Project related items and in Shepherd programme is indicated by a pass and is not taken into account for computing OPM.

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 90 credits. The student has acquired 10 more compulsory credits from Project and Shepherd courses. The student has also acquired _____ (if any) extra credits from courses offered by the parent department.

COURSE DETAIL

Sem.	Code	Course Title	Hrs/Wk	Credits
I	10PCH1101	Organic Chemistry I	6	5
	10PCH1102	Inorganic Chemistry I	6	5
	10PCH1103	Physical chemistry I	6	5
	10PCH1201 10PCH1202	Core Elective I A: Instrumental Methods of Analysis / B: Pharmaceutical Chemistry	4	4
	10PCH1104	Organic Chemistry Practical I	4	3
	10PCH1105	Physical Chemistry Practical	4	3
	Total for Semester I		***30***	***25***
II	10PCH2106	Organic Chemistry II	6	5
	10PCH2107	Inorganic Chemistry II	6	5
	10PCH2108	Physical Chemistry II	6	5
	10PCH2109	Inorganic Chemistry Practical I	4	3
	10PCH2301	Additional Core - Electrochemistry Practical	4	3*
	10PCH2401	HEALTH CHEMISTRY – IDC	4	4
	Total for Semester II		***30***	***22***
III	10PCH3110	Organic Chemistry III	6	5
	10PCH3111	Inorganic Chemistry III	6	5
	10PCH3112	Physical Chemistry III	6	5
	10PCH3113	Organic Chemistry Practical II	4	3
	10PCH3114	Inorganic Chemistry Practical II	4	3
	10PCH3402	INDUSTRIAL CHEMISTRTY – IDC	4	4
	Total for Semester III		***30***	***25***
IV	10PCH4115	Organic Chemistry IV	6	5
	10PCH4116	Inorganic Chemistry IV	6	5
	10PCH4203 10PCH4204	Core Elective II A: Analytical methods/ B: Essentials of Chemistry	4	4
	10PCH4205 10PCH4206	Core Elective III A: Thermodynamics / B: Organometallics for Organic Synthesis	4	4
	10PCH4501	Project	10	5*
	Total for Semester IV		***30***	***18***
I– IV	SHEPHERD		70	5*
Total minimum Credits				**90**

IDC offered from the Department of Chemistry to other department students:

II	08PCH2401	IDC – I Health Chemistry	4	4
III	08PCH3402	IDC – II Industrial Chemistry	4	4

Compulsory Extra credits (Project – 5, Shepherd-5)		**10**
1-4	**Total minimum credits**	**90**
Total credits		**100**

Extra Credits

2	10PCH2301	Electrochemistry practical	3

*Additional Credits (3 + 5 + 5 =13) ** Inter Departmental Course

Sem: I *Hours: 6*
Code:10PCH1101 *Credits: 5*

ORGANIC CHEMISTRY I

Objectives

1. To learn the concept of bonding, structure and reactivity of organic molecules
2. To understand the chemistry of heterocyclics and natural products

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-steric effects and strengths of acids and bases. Bonding weaker than covalent bond-addition compounds-Electron donor-acceptor complexes-Crown ether complexes and applications-Inclusion compounds, Clathrates-Catenanes and rotaxanes. Acids and Bases-introduction-Bronsted and Lewis acid-base concepts-pH, pKa and pKb scales

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

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- Altermant and non-altermant hydrocarbons-antiaromtic compounds-paratropic compounds. Aromatic characterization of azulenes, tropones, annulenes and fullerenes.

Unit III Reactive Intermediates

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

Free-radical substitution reactions- Mechanisms in aliphatic and aromatic substratesNeighbouring group assistance-Orientation and reactivity-Some selected reactionsHunsdieker, Kolbe, Meerwein arylation, and Hofrnann-Loffier-Fretag.

Unit IV Aromatic electrophilic and nucleophilic substitutions

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

Aromatic Electrophilic substitution - Arenium ion mechanism-Selected reactions – Reactivity-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.

Unit V Heterocyclics, Flavonoids and Anthocyanidines

Nomenclature – acyclic , alicyclic , bicyclic, spirocyclic compounds. Chemistry of 5-membered heterocyclic compounds containing one and two heteroatom (1,2&1,3). Structures and numbering of diazins (pyrazine, pyrimidine and pyrazine), azines (oxazine and azepine). Flavonoids-Anthocyanidin-chemistry of cyanidine-Flavone-synthesis of flavone-flavonol and quercetin-isoflavone-synthesis of daidzein.

TEXTS:

1. March J, *Advanced Organic Chemistry,* Fourth Edition, John-Wiley and Sons, New York (1992). Unit – I,II, III & IV
2. Eliel E L, *Stereochemistry of Carbon Compounds,* Tata-McGraw Hill Publishing Company, New Delhi (1998). Unit - I
3. Nasipuri D, *Stereochemistry of Carbon Compounds,* Second Edition, New-Age International Publishers, New Delhi (1996). Unit – I
4. Garratt P.J, Aromaticity, Unit – II
5. Finar, I.L, *Organic Chemistry Volume* 2, Sixth Edition, ELBS with Longmann, Singapore (1997). Unit – V

References:

1. Sykes P, *Guide Book to Mechanism in Organic Chemistry,* Sixth Edition, ELBS with Longmann (1997).
2. G.M.Badger G.M, Aromaticiy

Sem: I *Hours: 6*
Code:10PCH1102 *Credits: 5*

INORGANIC CHEMISTRY I

Objectives

1. To study the chemistry of transition and inner transition elements
2. To learn the principles and applications of nuclear reactions

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: Synthesis & Structure

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)], [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 reaction - 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 inalastic), fission, fusion- proportional counter, Geiger-Muller counter, scintillation counter and Cherankov counter. Accelerators- linear, cyclotron, synchrotron, betatron and bevatron.

Unit V: Nuclear Fission and Fusion and Applications of Trace Elements

Characteristics of fission reaction - product distribution, theories of fission -fissile and fertile isotopes, nuclear fusion and stellar energy, synthetic elements- Nuclear wastes-nuclear reprocessing-radiation hazards and prevention. Various atomic power projects in India - 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.

Texts

1. Lee J D, *Concise Inorganic Chemistry,* Sixth Edition, ELBS, London, 1998. Units - I, II, III
2. G. Friedlander *Nuclear and Radiochemistry* (Third Edition) John Wiley and Sons London (1990). Units - III, IV, V
3. Samuel Glasstone *Source book on Atomic energy* (Third Edition), New Delhi, Affiliated East West Press, Pvt. Ltd. Units - III, IV, V

REFERENCES

1. Cotton F A and Wilkinson G, *Advanced Inorganic Chemistry,* Third Edition, John- Wiley and Sons, New York, 1988.
2. Huheey, J E, *Inorganic Chemistry: Principles of Structure and Reactivity,* Second Edition, Harper and Row, New York, 1972.
3. Arniker, *Essentials of Nuclear chemistry.*

Sem: I *Hours: 6*
Code: 10PCH1103 *Credits: 5*

PHYSICAL CHEMISTRY I

Objectives

1. To study the fundamentals and applications of classical mechanics and quantum chemistry
2. To learn the fundamentals and applications of statistical thermodynamics

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 L_x, L_y, L_z- Vectors - vector space - Euclidean space, Hermitian space, Hilbert space.

UNIT III: Basic Quantum Chemistry

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 -Translational, rotational and vibrational partition functions of diatomic molecules-Translational, rotational and vibrational partition functions of poly atomic molecules-Electronic partition function-Derivation of thermodynamic quantities E, S, A, H, G, K and C_p, C_v using partition function-Sackur-Tetrode equation-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-Symmetric and antisymmetric wave function-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, 3
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, 5
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:10PCH1201 *Credits: 4*

CORE ELECTIVE I
A-INSTRUMENTAL METHODS OF ANALYSIS

Objectives

1. To study the analytical techniques, instrumentation and applications
2. To understand the principles and techniques of green chemistry

UNIT I ERROR ANALYSIS

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 & 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- the normal error curve – testing of significance- F- test & t- test – confidence limit- rejection of result –Dean – Dixon Quotient test (Q-test)- method of least square and correlation methods.

UNIT II CHROMATOGRAPHY

Principle of chromatography- retardation factor- classification of chromatographic techniques- partition chromatography: liquid-liquid, paper, gas-liquid chromatography – Adsorption chromatography: Column chromatography- Theory- procedure –applications - Thin layer chromatography: Principle - advantages – preparation of TLC plates- development of chromatogram - Affinity Chromatography and its uniqueness, Ion Exchange Chromatography- principle – applications: separation of amino acids rare earth elements- size exclusion chromatography - and HPLC- instrumentation- procedure and applications.

UNIT III THERMOANALYTICAL METHODS

Thermogravimetic analysis: Principle, thermal analysis of silver nitrate methods of obtaining thermogram - Derivative Thermogravimetry – Factors affecting thermograms- TGA instrumentation – Applications of TGA- Differential Thermal Analysis- DTA instrument- Applications: calcium oxalate monohydrate, calcium acetate, copper sulphate pentahydrate. Instrumentation and application of DSC

Unit IV SPECTROMETRIC METHODS

Colorimetry - fundamental laws - photoelectric colorimetry - different monochromators and detectors- applications- Fluorimetry and phosphorimetry - principle, applications - Flame photometry and atomic absorption spectrometry-principle and applications.

UNIT V GREEN CHEMISTRY

Introduction - Basic principles of green chemistry –Tools of Green Chemistry –Atom economy, Reactions of atom economy- Green solvents – Green reactions - Microwave Induced Green Synthesis: Introduction – water based reactions (only)- Nanotechnology- Synthesis of Carbon Nano Tubes (CNTs)- Types-Properties and uses.

Text books

1. U N Dash, *Analytical Chemistry – Theory and Practice*, 2nd Edn., Sultan Chand & Sons, New Delhi, *2005*.
2. Vogel A I, *A Text Book of Quantitative Inorganic Analysis*, 3rd Edn., London, Longman Group Ltd.
3. R Gopalan, P S Subramanian, K Rengarajan, *Elements of Analytical Chemistry*, 3rd Edi., Sultan Chand & Sons, New Delhi, *2003*.
4. Anastas P T; Warner JC; Green Chemistry: theory and Practice, Oxford University Press, New York, *1998.*

REFERENCES

1. R A Day & AL Underwood, *Quantitative Analysis*, 6th Edn., PHI, *2001*.
2. Gary A Christian, *Analytical Chemistry*, 6th Edn., John Wiley & Sons Ltd., *2003*.
3. P C Kamboj, *University Practical Chemistry*, Vishal Pub., Jalandhar, *2008.*
4. Willard and others, *Instrumental methods of analysis,* Third edition, East West Press, 1977
5. VK Ahluwalia, M Kidwai, *New Trends in Green Chemistry*, 2nd Edn, Anamaya Pub. New Delhi, *2006.*

Sem: I *Hours: 4*
Code:10PCH1202 *Credits: 4*

CORE ELECTIVE I
B-PHARMACEUTICAL CHEMSITRY

Objectives

1. To learn the chemistry of drugs and drug action
2. 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:

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

Sem: I *Hours: 4*
Code:10PCH1104 *Credits: 3*

ORGANIC CHEMISTY PRACTICAL I

Objectives

1. To learn the separation of binary organic mixtures and characterize them
2. 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: 10PCH1105 *Credits: 3*

PHYSICAL CHEMISTRY PRACTICAL-I

Objective

1. To learn some non-electrical physical chemistry experiments

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 – *p*-nitrotoluene 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/ oxalic 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: II *Hours: 6*
Code: 10PCH2106 *Credits: 5*

ORGANIC CHEMISTRY II

Objectives

1. To understand the stereochemistry and its implications in molecular dynamics
2. To probe the addition, elimination, reduction 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-SN1 and SN2 - formation and cleavage of epoxide rings-addition reactions to double bonds-electrophilic addition-nucleophilic addition-*cis* addition via cyclic intermediate- E2 eliminations-pyrolytic *cis* - elimination-l ,4-elimination leading to molecular fragmentation. Stereochemistry of Diels-Alder Reactions.

General reactions with reference to stereochemistry-chromic acid oxidation of cyclohexanols-Neighbouring group participation-

participation of intemal nucleophile and p-electrons of double bonds. Deamination of 2-amino cyclohexanols. Stereoselective and stereo specific reactions. Asymmetric synthesis and asymmetric induction-addition of nucleophiles to carbonyl compounds - Crams's rule

Carbohydrates-ring structures-Determination of configuration of monosaccharidesconfiguration of C1 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 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-Taft equation and its applications.

UNIT III Aliphatic nucleophilic and electrophilic substitutions

Aliphatic nucleophilic substitution SN1 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 SE1 and SE2and 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 IV : 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-E1, E2 and E1cBmechanisms-spectrum of E1, E2 and E1cB mechanisms, orientation and reactivity. Bredt's rule. Selected reactions-dehydration of alcoholsdehydrohalogenation-Chugeaev reaction-Hofmann exhaustive methylation-Cope elimination-Shappiro reaction. Extrusion Reactions

UNIT V: 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- Swern and Dess-Martin oxidations - catalytic hydrogenation and dehydrogenation- Synthetic uses of the following reductants NaNH2, Wilkinson's catalyst, LAH, NaBH4, (*t*-BuO)3AlH, NaBH3CN, R3SnH, Me3SiCN, alkali metals, hydrazine. MPV reduction.

TEXT BOOKS:

1. Eliel E L, *Stereochemistry of Carbon Compounds,* Tata-McGraw Hill Publishing Company, New Delhi (1998). Unit – I
2. Finar I L, *Organic Chemistry* Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997). Unit – V
3. Sykes P, *Guide Book to Mechanism in Organic Chemistry,* Sixth Edition, ELBS with Longmann (1997). Unit – II
4. March J, *Advanced Organic Chemistry,* Fourth Edition, John-Wiley and Sons, New York (1992). Unit – III & IV

5. House. H.O. "Modern Synthetic reactions", W.A. Benjamin Inc, New York, (1980), Unit - V.

REFERENCES

1. Mackie R.K & Smith D.M, Guide book of organic synthesis
2. Kalsi P S, *Stereochemistry: Conformation and Mechanism,* 4th Edition, NewAge International Publishers, New Delhi (1997).
3. Clayden, J et al. Organic Chemistry , Oxford university press, 2005

Sem: II *Hours: 6*
Code:10PCH2107 *Credits: 5*

INORGANIC CHEMISRY II

Objectives

1. To understand the hybridization, bonding and structures of inorganic compounds
2. to understand the periodicity of the 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 - 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 and ions such as BeH_2 and NO_2^-. VSEPR theory – methane, ethylene, acetylene, ammonia, water, PCl3F2 (Bent's rule), SF_4, BrF_3, TeF_5^-, ICl_2^-, ICl_4^-, XeF_2, XeF_4, XeF_6, XeO_3, XeO_4, phosphorus trihalides bond angle, ammonia & NF3 dipole moments, H_2O, OF_2 angle, NH_3, XeO_3 angle, 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-Hard and soft acids and bases - acid base strength and hardness and softness

- symbiosis. Theoretical basis of hardness and softness, electronegativity and hardness, softness. Types of solvents, types of reactions - autoionisation and neutralisation, precipitation, solvation, solvolysis, complex formation-*Liq.* NH_3, alkali metals in *liq.* NH_3, SO_2, HF and H_2SO_4 as solvents.

UNIT IV Periodicity, 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 – bonding in noble gas fluorides and their reactivity

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, ultramarines – 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 bondstructure of B_2H_6, B_4H_{10}, $[B_{12}H_{12}]^{2-}$,B_6H_{10}, B_8H_{12}, $B_{10}H_{14}$, *closo*, *nido*, *arachno* boranes and carboranes- - Silicones-preparation, properties and uses.

TEXT

1. Huheey J.E., *Inorganic Chemistry*, (Second Printing) New york, Harper & Row publishers (1972). All the five units

REFERENCES

2. Cotton F.A. and Wilkinson G., *Advanced inorganic chemistry,* (Third Edition) London, John Wiley & Sons (1988).

3. Sisler *Chemistry of Non- aqueous solvents.*

Sem: II *Hours: 6*
Code: 10PCH2108 *Credits: 5*

PHYSICAL CHEMISTRY II

Objectives

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

UNIT 1 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

1. Drago.R.S *Physical methods in inorganic chemistry* New Delhi, East West Press Ltd, (1971).
2. Chang. R *Basic principles of spectroscopy* New Jersy, Englewood Cliffs (1978).
3. Straughan.B.P and Walker.S *Spectroscopy Voll,2,3,* New York, London Chapman and Hall, A Halstet Press Book, John Wely & Sons Ins. 1975).
4. G.M.Barrow, *Introduction to Molecular spectroscopy,* Tata McGraw - Hill Edition (1993).

Semester II *Hours: 4*
Code:10PCH2401 *Credits: 4*

HEALTH CHEMISTRY

Objectives:

1. To know the essentials of health, drugs
2. To learn the functions of enzymes, hormones and body fluids
3. 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.

Texts

1. Jayashree Ghosh, A Text book of Pharmaceutical Chemistry, S. Chand and Co.Ltd, 1999.UNITS II and V
2. Alex V Ramani, Food Chemistry, MJP Publishers, Chennai, 2009 UNIT I
3. Deb A C, Fundamentals of Biochemistry, New Central Book Agency, Calcutta, 1994. UNIT III
4. Satake M and Mido Y, Chemistry for Health Science, Discovery Publishing House, New Delhi, 2003. UNIT I and III

References

1. Ashutosh Kar, Medicinal Chemistry, Wiley Easterns Limited, New Delhi, 1993 UNIT II & IV

Sem: II *Hours: 4*
Code:10PCH2109 *Credits: 3*

INORGANIC CHEMISTRY PRACTICAL I

Objectives

1. To learn the qualitative analysis of common metals and rare metals
2. To learn colorimtric analysis
3. To learn to prepare inorganic complexes

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: II *Hours: 4*
Code: 10PCH2301 *Credits: 3*

ADDITIONAL CORE ELECTROCHEMISTRY PRACTICAL

Objectives

1. To learn some conductometric and potentiometric titrations

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: III *Hours:6*
Code:10PCH3110 *Credits: 5*

ORGANIC CHEMISTY III

Objectives

1. To understand the spectroscopic techniques in the structure determinations
2. To enumerate the various synthetic strategies of organic molecules

UNIT I: 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, a,b-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, a-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: Spectroscopy II

PMR spectroscopy-chemical shift-magnetic non equivalence of protons-types of coupling and coupling constants (*J1, J2* - 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 C-C bonds-reactions of organometallic compounds- Palladium based reactions: Heck reaction, Suzuki coupling, Stille coupling, Hiyama coupling - 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 Li, 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*-Bu3SnH, LDA, baker yeast, Me2CuLi (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 & 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-*p* methane reaction

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-photochemistry of alkenes, dienes, carbonyl compounds and aromatic compounds-photoaddition.

TEXT BOOKS

1. Silverstein R M and Bassler G C, *Spectrometric Identification of Organic Compounds,* Fourth Edition, John- Wiley and Sons, New York (1993). Unit – II
2. Norman R.O.C., & Co., on J.M. Principles of Organic Synthesis 2nd Edition, ELBS (1986) Unit III & IV
3. Depuy C.H & Chapman, Molecular reactions and photochemistry, Prentice Hall of India, New Delhi, Unit – V
4. Woodward R.B & Hoffman R, The conservation of orbital symmetry, Unit – V

REFERENCES:

1. Dyer J.R, Applications of absorption spectroscopy of Organic compounds.

2. Sharma Y.R, Elementary organic spectroscopy.

3. Fleming I, *Spectroscopic Methods in Organic Chemistry,* Fourth Edition, Tata-McGraw Hill Publishing Company, New Delhi (1988).

4. Stewart Warren, Designing Organic synthesis: The Disconnection Approach, Wiley, New Delhi, (1984)

5. Mackie R.K & Smith D.M, Guide book of organic synthesis.

6. Clayden J et al Organic Chemistry, Oxford University Press (2005).

Sem: III *Hours: 6*
Code:10PCH3111 *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 behaviours of complex compounds

UNIT I: Theories of Coordination Chemistry

Review of isomerism and limitations of VB theory - 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 bonds) – MO of Td 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. 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 base hydrolysis-mechanisms-evidences, trans effect -theories and Applications- Electron transfer reaction mechanisms-Catalysis by organometallic compounds-oxidativeaddition-insertion-hydrogenation-hydoformylation-Wacker process, Fischer-Tropsch reaction, Zeigler-Natta Catalyst, Wilkinson's catalyst.

UNIT IV: Physical Methods in Coordination Chemistry I

Types of magnetic behaviour - magnetic susceptibility measurements-Guoy 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-Infra red spectra of Coordination complexes-characteristic frequencies-mode of coordination and interpretation of ClO_4^-, SO_4^{2-}, CO_3^{2-}, ester, amine, amide groups using IR spectra.

UNIT V: Physical Methods in Coordination Chemistry II

NMR – applications of NMR to inorganic compounds (19F and 31P 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_3CO_{12}, $I_2Cl_4Br_2$.

TEXTS

1. Ebsworth EAV; *Structural Methods in Inorganic Chemistry*, 3rd Ed, Great Britain, ELBS, 1987. Units - III, V
2. Drago R S; *Physical Methods in Chemistry*, 3rd Ed., Philadelphia, London, W. B. S. Saunders Company, 1992. Units - IV, V
3. Basalo F and Pearson R G, *Mechanisms of Inorganic Reactions,* John-Wiley and Sons Inc., New York (1960). Unit III
4. Cotton F.A. and Wilkinson G~, *Advanced inorganic chemistry,* (Third Edition) London, John Wiley & Sons (1988). Units - I, II, III, IV

5. Huheey, J.E., Inorganic Chemistry Refer Page 33 Text 1 1-IV Units.

REFERENCES

1. Lewis J and Wilkins R G, *Modern Coordination Chemistry,* Interscience Publishers, Inc., New York (1960).
4. Sutton, *Electronic spectra of Coordination compounds.*
5. Nakamota, *IR Spectral Identification of Inorganic compounds*
6. Straughn B P; Walker S*; Spectroscopy* Vol., London, Chapman & Hall, 1976.
7. Gibbs T C; *Principles of Massbauer Specroscopy*, London, Chapman & Hall, 1976.

Sem: III *Hours: 6*
Code: 10PCH3112 *Credits: 5*

PHYSICAL CHEMISTRY III

Objectives

1. To understand the theories of kinetics of reactions and catalysis
2. To understand the kinetics and the theories 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 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). Units - I, II, III
2. Kuriacose and Rajaram, *Kinetics and Mechanism of chemical transformation,* Macmillan &Co (1993). Units - I, II, III
3. L. Antorpov, *Theoritical Electrochemistry,* Mirpublishers, Mascow. Units - IV, V
4. Glasstone.S *An Introduction to electrochemistry,* New Delhi, East West Press Pvt. Ltd, (1956). Units - IV, V

REFERENCS

1. Bockris J O'M and Reddy A K N, *Modern Electrochemistry Vol 1 & 2,* Second Edition, Plenum Press, New York (1998).
2. G. Hughes, *Radation Chemistry,* Oxford ser ies (1973).

Semester III *Hours: 4*
Code: 10PCH3402 *Credits: 4*

INDUSTRIAL CHEMISTRY

Objectives:

1. To learn some of the Industrial products and their manufacturing processes
2. To become aware of the applications of the Industrial products

UNIT I Cement and Ceramics

Cement – Composition, types – Portland cement – Composition, types, manufacture (Wet and Dry process), uses – Setting of cement; Ceramics – Composition, Classification, manufacture, properties and uses

UNIT II Glass and Matches

Glass- Composition, Types, Formation operations – Melting, Blowing, Pressing, Annealing and finishing; Matches – Composition, Types, Manufacture – safety matches

Unit III Pigments, Dyes and Paints

Pigments – Classification, Manufacture and uses; Dyes – Classification, preparation, Dyeing processes; Paints – Composition, Types, Manufacture and testing of Paints

Unit IV Plastics and Fibres

Fibres – Natural and synthetic fibres, Artificial silk, rayon, nylon and trylene; Plastics – composition, Classification, manufacture, properties and uses

Unit V Fertilizers and Fuels

Fertilizers – Organic and Inorganic fertilizers, Preparation and uses

Fuels – Energy resources - Industrial gases, Water gas, Producer gas, Oil gas, natural gas, coal gas, Gobar gas, Indane gas, Petroleum products and coal products.

TEXTBOOKS

1. Charkarabarthy B.N, Industrial Chemistry, Oxford and IBH Prb.Co. IV AND V
2. Sharma B.K, Industrial Chemistry, Goel Publishing House. ALL THE FIVE UNITS

REFERENCES

1. Kirk Othmer, Encyclopedia of Chemical Technology. ALL THE FIVE UNITS

Sem: III *Hours: 4*
Code:10PCH3113 *Credits: 3*

ORGANIC CHEMISTY PRACTICAL II

Objectives

1. To learn quantitative analysis in organic chemistry
2. To learn some double stage organic preparations
3. 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: III *Hours: 4*
Code:10PCH3114 *Credits: 3*

INORGANIC CHEMISTRY PRACTICAL II

Objectives

1. To learn quantitative separation of metal ions in binary mixtures
2. 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 μ_{eff} of a complex by Guoy 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)

Sem: IV *Hours: 6*
Code:10 PCH 4115 *Credits: 5*

ORGANIC CHEMISTRY IV

Objectives

1. To understand electroorganic reactions
2. To understand the chemistry of hormones, nucleic acids and other natural prouducts
3. To study named organic reactions and rearrangements

UNIT I Electroorganic Reactions & Hormones

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.

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 II 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

UNIT III Alkaloids, Terpenoids, Antibiotics and Vitamins

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

Terpenoids- introduction-extraction-classification-commercial and

medicinal values-structural elucidation of zingiberene-biosynthesis of terpenoids.

Antibiotics - structural elucidation of chloramphenicol-structure and functions of penicillin, streptomycin and terramycin. .

Vitamins - structure and functions of Vitamins A1, A2, A3, B, B12, C, E and K (structural elucidations not required).

UNIT IV Nucleic acids and proteins

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) - replication of DNA - genes genetic code and informational theory. Proteins - Amino acid synthesis-peptide synthesis-End group analysis-secondary structure of proteins

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.

TEXT BOOKS

1. Rifi &Covitz, Introduction to organic electrochemistry, Uint- I
2. Mayo P. de "Molecular rearrangement", Unit - II
3. Finar I L, *Organic Chemistry* Volume I and II, 6th Edi., ELBS with Longmann, Singapore (1997). Uint- I, III &IV
4. March J, *Advanced Organic Chemistry;* Fourth Edition, John-Wiley and Sons, New York (1992). Uint- II &V

REFERENCES

1. Clayden J et al. Organic chemistry, oxford university press, 2005
2. Carey, F.A., & Seendberg R.J., Advanced Organic Chemistry.

Sem:IV *Hours: 6*
Code:10PCH4116 *Credits: 5*

INORGANIC CHEMISTRY IV

Objectives

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

UNIT I : Elements of Solid State

Elements of crystallography - space lattices-unit cells-crystal system- 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, ReO_3 structure - spinels and anti spinels- covalent crystals diamond and graphite – Crystal Structure & properties.

UNIT II: Theories and structures of solids

Crystal defects-point, line and plane defects- colour centers- non-stoichiometric compounds-Electronic structure of solids- free electron and band theory of solids. Types of solids - electrical conductivity and superconductivity - high temperature superconductors-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.

Unit III : Bio-inorganic Chemistry I

Essential, non-essential and toxic elements – Egamic hypothesis – toxicity of metal ions - Ion transport mechanism in cell membrane-Na and K pumps-ionophores-Metal ion interaction with nucleic acids

-metal ions and DNA functions- replication, transcription and translation- Blue copper proteins- metal based drugs-Nitrogen Fixation- in vivo & in vitro.

Unit IV : Bio-inorganic Chemistry II

Transition metal ions in biology - Structure and characteristic features of heamoglobin and myoglobin - Chlorophyll, Mechanism, role of Mn in Photosynthesis - Cytochromes Electron transfer reactions - Synthetic oxygen carriers - vitamin B12

Unit V : Photochemistry

Basic laws of Photochemistry-Photo physical processes-Photo chemical primary processes- rate constant and life time of reactive energy states - types of photochemical reactions-Photo chemistry of transition metal complexes- photo redox, substitution and exchange reactions-light induced isomerisation, dissociation and linkage isomerisation reactions-Photochemistry of organometallic compounds and Cr and Ru complexes.

TEXTS

1. *Eichron,G.L Inorganic Biochemistry,* New York, Elsevier publications (1975). Units - III, IV
2. Azaroff *Introduction to solids* New Delhi Tata McGraw Hill Publishing Co., (1994). Units - I, II
3. Evans,R.C *Crystal Chemistry* England, C.U.Press(1964). Units - I, II
4. Rohatgi Mukherjee, Fundamentals of photochemistry, New Delhi. Unit - V

REFERENCES

1. Addison, W.E *Structural Principles of inorganic compounds,* UK Longmans Publications (1961).
2. Lipson *Determination of Crystal Structures* (volume 3) New York Bell Publications (1953).

3. Rao, C.N.R *Solid State Chemistry,* New York, Marcel & Dekker Inc., (1974).

4. Rao, C.N.R *Phase Transitions in Solids,* New York, McGraw-Hill Co., (1978).

5. Keer, H.V *Principles of Solid State,* New Delhi, Wiley Eastern Ltd., (1993).

6. Arora *Solid State Chemistry,* New Delhi, Anmol Publications (1980).

Sem: IV Hours:4
Code: 10PCH4203 Credits: 4

CORE ELECTIVE II
A- ANALYTICAL METHODS

Objectives

1. To understand the electro-analytical techniques, instrumentation and applications
2. To understand the concepts and applications of quantum chemistry and NQR and Mossbauer spectroscopy
3. To understand the kinetics of polymerization and the physical properties of polymers

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 I

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 II

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 al., *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: 10PCH4204 *Credits: 4*

CORE ELECTIVE II
B - ESSENTIALS OF CHEMISTRY

Objectives

1. To be able to solve the problems in quantum chemistry, spectroscopy, transition elements, functional group interconversions and photochemical reactions

Concepts and problems in topics in the following five units

Unit I

Quantum theory –principles and techniques – applications to a particle in a box – Harmonic oscillator

Rigid rotor – Hydrogen atom – VB theory- MO theory –symmetry

Unit II

Spectroscopy – Molecular NMR , ESR, NQR and Moss Bauer spectroscopy- instrumental methods of analysis- spectrophotometeric and electro analytical methods- kinetic theory of gases- rates of reactions – temperature dependence of chemical reactions- consecutive reactions- steady state approximation – homogeneous and heterogeneous catalysis.

Unit III

Non transition elements- characteristics- structure and reactions of compounds- boranes- silicates- oxoacids pf N, P, S and halogens – xenon compounds – structure of NaCl , CsCl, diamond and graphite- band theory in semiconductor – transition elements- general characteristics of d and f block elements- structure , stability reactions and spectra and magnetism of coordination compounds of 3d block elements – LF theory – simple organometallic compounds – role of metals in biological systems.

Unit IV

Reactions, synthesis and mechanism involving the following alkynes, arenes, alcohol, phenol, carbonyl compounds, acids, their derivatives, halides, nitrocompound, amines, stereo chemical and conformational analysis of above compounds leading to specific reactivity.

Unit V

Principles of photochemical excitation- photochemistry of olefins and carbonyl compounds- cycloadditions, electrocyclic and sigmatropic shifts- Woodward Hofmann rule, molecular rearrangements involving electron deficient atoms- carbohydrates, hetrocyclics (thiopene, furan, pyrrole, pyridine)-reactions – structure- properties of mono and disaccharides.

TEXTBOOKS

1. Morrison, R.T, Boyd, R.N(Fourth Edition)Sydney Allyn& Bacon Inc.,(1983). Units - IV, V
2. Lee,J.D . Concise Inorganic chemistry England ELBS Ltd (1978). Unit - III
3. Atkins, P.W Physical chemistry (Fourth Edition) London ELBS Ltd (1994). Units - I, II

References

1. March J, advanced organic chemistry New York John Wiley& Sons (1999).
2. Huheey, J.EE.A.Keitler, R.L India Pearson education Asia private Ltd., (2000).
3. Adamson, A.W Understanding physical chemistry (Vol 1and 2) New York, W.A.Benjamin Inc.,(1964).
4. Atkins, P.W and Pratt solutions to problems in physical chemistry, Oxford university press (1994).

Sem:IV *Hours: 4*
Code: 10PCH4205 *Credits: 4*

CORE ELECTIVE III A-THERMODYNAMICS

Objectives

1. To understand the equilibrium and non-equilibrium thermodynamics
2. To inculate interest in solving thermodynamic problems
3. To study the experimental techniques to measure the thermodynamic quantities

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 - 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 II: Chemical Thermodynamics II and Near Equilibrium Thermodynamics I

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.

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 $L_{l2} = L_{21}$)

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 - $L_{l2} = L_{21}$ by transference number method - Irreversible thermodynamics and biological systems.

UNIT V: Numerical Problems and Experimental Methods 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 - III law of thermodynamics - Thermochemistry-Kirchoff's equation

Experimental methods used in thermodynamics - Determination of DH, DS, DG - determination of heat of mixing and volume of mixing - Adiabatic compressibility (ultrasonic interferometer) - Bomb Calorimeter - Vapour pressure by isoteniscope method

TEXT BOOKS

2. 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).

Sem: IV *Hours: 4*
10PCH4206 Credits: 4

B-ORGANOMETALLICS FOR ORGANIC SYNTHEIS

Objectives

1. To know the structure and reactivity of organometallic reagens
2. To study the applications of various organometallics in organic synthesis

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

TEXTBOOKS

1. Swan N M and Black D S T C. Organometallics in organic synthesis, NewYork, John-Wiley (1974). ALL THE FIVE UNITS

REFERENCES

1. Coates G E, Loff Green, Powell Kowade P. Principles of organometallic chemisty, Second Edition, ELBS with Chapmann and Hall (1988) ALL THE FIVE UNITS
2. Mehrotra Anirudh Sigh R C. Organometallic chemistry, Wiley-Eastern Limited, NewDelhi (1991) ALL THE FIVE UNITS

INTER DEPARTMENTAL COURSE - IDC

BIOCHEMISTRY

10PBC2401 APPLIED NUTRITION

10PBC3402 FIRST AID MANAGEMENT

BIOTECHNOLOGY

10PBT2401 BASIC BIOINFORMATICS

10PBT3402 BASIC GENOMICS & PROTEOMICS

CHEMISTRY

10PCH2401 HEALTH CHEMISTRY

10PCH3402 INDUSTRIAL CHEMISTRY

COMMERCE

10PCO2401 FINANCIAL ACCOUNTING FOR MANAGERS

10PCO3402 MANAGEMENT CONCEPTS & ORGANIZATIONAL BEHAVIOR

COMPUTER APPLICATIONS

10PCA2401 INTERNET CONCEPTS

10PCA2402 FOUNDATION OF COMPUTER SCIENCE

10PCA3403 COMPUTER APPLICATIONS FOR SOCIAL SCIENCES

10PCA3404 FUNDAMENTALS OF PROGRAMMING

COMPUTER SCIENCE

10PCS2401A FUNDAMENTALS OF IT

10PCS2401B WEB DESIGN

10PCS3402A FLASH

10PCS3402B DREAM WEAVER

ECONOMICS

10PEC2401 ECONOMICS FOR MANAGERS

10PEC3402 INDIAN ECONOMY

ELECTRONICS

10PEL2401 ELECTRONICS IN COMMUNICATION

10PEL3402 COMPUTER HARDWARE

ENGLISH

10PEN2401 BUSINESS ENGLISH

10PEN3402 INTERVEIW SKILLS AND GROUP DYNAMICS

HISTORY

10PHS2401 PUBLIC ADMINISTRATION

10PHS3402 APPLIED TOURISM

HUMAN RESOURCE MANAGEMENT

10PHR2401 FUNDAMENTALS OF HRM

10PHR3402 PERSONALITY AND SOFT SKILLS DEVELOPMENT

INFORMATION TECHNOLOGY

10PIT2401A FUNDAMENTALS OF IT

10PIT2401B WEB DESIGN

10PIT3402A FLASH

10PIT3402B DREAM WEAVER

MATHEMATICS

10PMA2401 OPERATIONS RESEARCH

10PMA3402 NUMERICAL METHODS

PHYSICS

10PPH2401 MODERN PHOTOGRAPHY

10PPH3402 MEDICAL PHYSICS

PLANT BIOLOGY & PLANT BIOTECHNOLOGY

10PPB2401 NANOBIOTECHNOLOGY

10PPB3402 REMOTE SENSIND AND GIS

TAMIL

10PTA2401 muRg gzpj NjuTj jkpo - 1

10PTA3402 muRg gzpj NjuTj jkpo - 2