M. Sc. CHEMISTRY SYLLABUS - 2014

SCHOOLS OF EXCELLENCE with CHOICE BASED CREDIT SYSTEM (CBCS)



SCHOOL OF PHYSICAL SCIENCES St. JOSEPH'S COLLEGE (Autonomous)

Accredited at 'A' Grade (3rdCycle) by NAAC College with Potential for Excellence by UGC **TIRUCHIRAPPALLI - 620 002, INDIA**

SCHOOLS OF EXCELLENCE WITH CHOICE BASED CREDIT SYSTEM (CBCS)

POST GRADUATE COURSES

St. Joseph's College (Autonomous), a pioneer in higher education in India, strives to work towards the academic excellence. In this regard, it has initiated the implementation of five "Schools of Excellence" from this academic year 2014 - 15, to standup to the challenges of the 21st century.

Each School integrates related disciplines under one roof. The school system allows the enhanced academic mobility and enriched employability of the students. At the same time this system preserves the identity, autonomy and uniqueness of every department and reinforces their efforts to be student centric in curriculum designing and skill imparting. These five schools will work concertedly to achieve and accomplish the following objectives.

- Optimal utilization of resources both human and material for the academic flexibility leading to excellence.
- Students experience or enjoy their choice of courses and credits for their horizontal mobility.
- The existing curricular structure as specified by TANSCHE and other higher educational institutions facilitate the Credit-Transfer Across the Disciplines (CTAD) a uniqueness of the choice based credit system.
- Human excellence in specialized areas
- Thrust in internship and / or projects as a lead towards research and
- The **multi-discipline** nature of the newly evolved structure (School System) caters to the needs of stake-holders, especially the employers.

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 correlation between credits and hours. 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 110 credits. The total number of courses offered by a department is given above. However within their working hours few departments/School can offer extra credit courses.

SUMMARY OF HOURS AND CREDITS PG COURSES - CHEMISTRY

Part	Semester	Specification	No. of Courses	Hours	Credits	Total Credits
1	I-IV	Core Courses				
		Theory	10	80	67	
		Practical	6			
	П	Self Paced Learning	1	-	2	
	Ш	Common Core	1	6	5	81
	IV	Comprehensive Examination	1	-	2	
	īV	Dissertation & Viva Voce	1	10	5	
2	III-IV	Core Electives	3	12	12	12
3	I-III	IDC (WS)	1	4	4	
		IDC (Common)	1	4	4	12
		IDC (BS)	1	4	4	
4	I-IV	Additional Core Courses	-		-	
5	ĪV	SHEPHERD & Gender Studies	1	-	5	5
		TOTAL		120		110

- IDC Inter Departmental Courses
- BS Between School
- WS Within School
- Total Hours : 120
- Total Credits : 110

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Course Pattern

The Post Graduate degree course consists of five vital components. They are cores courses, core electives, additional core courses, IDC's and SHEPHERD. Additional Core courses are purely optional on the part of the student. SHEPHERD, the extension components are mandatory.

CORE COURSE

A core course is the course offered by the parent department related to the major subjects, components like theories, practicals, self paced learning, common core, comprehensive examinations, dissertations & viva voce, field visits, library record form part of the core courses.

CORE ELECTIVE

The core elective course is also offered by the parent department. The objective is to provide choice and flexibility within the School. There are three core electives. It is offered in different semester according to the choice of the school.

ADDITIONAL CORE COURSES (If any)

In order to facilitate the students gaining extra credit, the additional core courses are given. The students are encouraged to avail this option of enriching with the extra credits.

INTER DEPARTMENTAL COURSES (IDC)

IDC is an interdepartmental course offered by a department / School for the students belonging to other departments / school. The objective is to provide mobility and flexibility outside the parent department / School. 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.

There are three IDC's. Among three, one is the Soft-Skill course offered by the JASS in the II Semester for the students of all the Departments. The other one is offered "With-in the school" (WS) and the third one is offered "Between the school" (BS). The IDC's are of application oriented and inter disciplinary in nature.

Subject Code Fixation

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

14	PXX	Х	Х	XX
\downarrow	\downarrow	\downarrow	\downarrow	\downarrow
Year of	PG Code of	Semester	Specification	Running number
Revision	the Dept	of the Part	of Part	in the part
14	PCH	1	1	01

For Example :

I M.Sc. Chemistry, first semester, Inorganic Chemistry-I The code of the paper is 14PCH1101.

Thus, the subject code is fixed for other subjects.

Specification of the Part

- 1. Core Courses: (Theory, Practical, Self paced Learning, Common Core, Comprehensive Examination, Dissertation and Viva-voce)
- 2. Core Electives
- 3. Additional Core Courses (if any)
- 4. Inter Departmental Courses (WS, Soft Skill & BS)
- 5. SHEPHERD & Gender Studies

EXAMINATION

Continuous Internal Assessment (CIA):

PG - Distribution of CIA Marks			
Passing Minimum: 50 Marks			
Library Referencing	5		
3 Components	35		
Mid-Semester Test	30		
End-Semester Test	30		
CIA 100			

MID-SEM & END-SEM TEST

Centralised – Conducted by the office of COE

- 1. Mid-Sem Test & End-Sem Test: (2 Hours each); will have Objective + Descriptive elements; with the existing question pattern PART-A; PART-B; and PART-C
- 2. CIA Component III for UG & PG will be of 15 marks and compulsorily objective multiple choice question type.
- 3. The CIA Component III must be conducted by the department / faculty concerned at a suitable computer centres.
- 4. The 10 marks of PART-A of Mid-Sem and End-Sem Tests will comprise only: OBJECTIVE MULTIPLE CHOICE QUESTIONS; TRUE / FALSE; and FILL-IN BLANKS.
- 5. The number of hours for the 5 marks allotted for Library Referencing/ work would be 30 hours per semester. The marks scored out of 5 will be given to all the courses (Courses) of the Semester.

SEMESTER EXAMINATION

Testing with Objective and Descriptive questions

Part-A: 30 Marks Objective MCQs only

Answers are to be marked on OMR score-sheet. The OMR score-sheets will be supplied along with the Main Answer Book. 40 minutes after the start of the examination the OMR score-sheets will be collected.

Part-B + C = 70 Marks

Descriptive

Part-B: $5 \ge 5 = 25$ marks; inbuilt choice; **Part-C:** $3 \ge 15 = 45$ marks; 3 out of 5 questions, open choice.

The Accounts Paper of Commerce will have **Part-A**: Objective = 25

Part-B: 25 x 3 = 75 marks.

Duration of Examination must be rational; proportional to teaching hours 90 minute-examination / 50 Marks for courses of 2/3 hours/week (all Part IV UG Courses) 3-hours examination for courses of 4-6 hours/week.

EVALUATION

Percentage Marks, Grades & Grade Points UG (Passing minimum 40 Marks)

Qualitative Assessment	Grade Points	Grade	Mark Range %)
Exemplary	10	S	90 & above
Outstanding	9	A+	85-89.99
Excellent	8	А	80-84.99
Very Good	7	В	70-79.99
Good	6	С	60-69.99
Pass (PG)	5	D	50-59.99
RA(PG)	0	RA	< 50

CGPA - Calculation

Grade Point Average for a semester is calculated as indicated here under:

Sum total of weighted Grade Points Sum of Gredits Weighted Grade Points is *Grade point x Course Credits*. The final CGPA will only include: Core, Core Electives & IDCs.

A Pass in SHEPHERD will continue to be mandatory although the marks will not count for the calculation of the CGPA.

POSTGRADUATE				
	Mark Range (%)			
CLASS	ARTS	SCIENCES		
Distinction	75 & above,	80 & above, first		
DISTINCTION	first attempt	attempt		
First	60 - 74.99	60 - 79.99		
Second	50 - 59.99	50 - 59.99		

Declaration of Result:

Mr./Ms	has successfully completed the Post Graduate			
in	programme. The candidate's Cumulative Grade Point			
Average (CGPA) is	and the class secured			
by completing the minimum of 110 credits.				

The candidate has also acquired ______ (if any) additional credits from courses offered by the parent department.

M. Sc. Chemistry

Course Pattern - 2014 Set

Sem	Code	Course	Hrs	Crs
I	14PCH1101	Inorganic Chemistry I	6	5
	14PCH1102	Organic Chemistry I	6	5
	14PCH1103	Physical Chemistry I		5
	14PCH1104	Organic Chemistry Practical I		3
	14PCH1105	Physical Chemistry Practical I		3
	14PCH1401	IDC: (WS) Industrial Products		4
		Total of Semester I		
	14PCH2106	Inorganic Chemistry II	6	5
	14PCH2107	Organic Chemistry II		5
	14PCH2108	Physical Chemistry II		5
п	14PCH2109	Organic Chemistry Practical II	4	3
"	14PCH2110	Physical Chemistry Practical II	4	3
	14PCH2111	Self Paced Learning - Analytical Chemistry	-	2
	14PSS2401	IDC : Soft Skill	4	4
		Total for Semester II	30	27
	14PCH3112	Inorganic Chemistry III	6	5
	14PCH3113	Organic Chemistry III	6	5
	14PPS3101	Common Core – Methods of Spectroscopy and Lasers	6	5
ш	14PCH3114	Inorganic Chemistry Practical I	4	3
	14PCH3201 A	Elective: Thermodynamics I OR	4	
	14PCH3201 B	Thermodynamics II	4	4
	14PCH3402	IDC : (BS) Health Chemistry	4	4
	Total for Semester III			26
	14PCH4115	Inorganic Chemistry IV	4	4
	14PCH4116	Organic Chemistry IV	4	4
	14PCH4117	Inorganic Chemistry Practical II	4	4
	14PCH4118	Comprehensive Examination	-	2
IV	14PCH4202 A	Elective : Physical Chemistry III OR	4	4
	14PCH4202 B	Polymer Chemistry	4	4
	14PCH4203 A	Elective: Natural Products OR	4	4
	14PCH4203 B	Pharmaceutical Chemistry	4	4
	14PCH4119	Dissertation & viva voce	10	5
		Total for Semester IV		32
I - IV	14PCW4501	SHEPHERD & Gender Studies	-	5
	Total for all Semesters			110

Sem. I 14PCH1101

Hours/Week: 6 Credits: 5

INORGANIC CHEMISTRY-I

Objectives

• To understand the chemistry of transition and inner transition elements.

- To know the fundamentals and instrumentation of nuclear chemistry.
- To understand the applications of nuclear chemistry.

Unit I:

Transition Elements

(16 Hours)

Transition elements - General characteristics - atomic, ionic radii - 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

(16 Hours)

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 - Gadalonium break, shift reagents - Extraction of thorium and uranium. Comparison of actinides and lanthanides.

Unit III:

Selected Compounds of d-block elements and fundamentals of nuclear chemistry (16 Hours)

Selected Compounds of d- block elements (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)], basic zinc acetate.

Fundamentals of Nuclear Chemistry

(16 Hours)

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

(16 Hours)

Q value of nuclear reaction, Coloumbic barrier, nuclear cross section, threshold energy and excitation function-Different types of nuclear reactions

with accelerated particles. Projectile capture and particles emission, spallation, fragmentation, nuclear fission, nuclear fusion- proportional counter, Geiger-Muller counter, scintillation counter and Cherankov counter. Linear accelerator, cyclotron, synchrotron.

Unit V:

Applications of Fission, Fusion and Trace Elements (16 Hours)

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 - Radio carbon dating - 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 14PCH1102

Hours/Week: 6 Credits: 5

ORGANIC CHEMISTRY-I

Objectives

- To learn the basic concepts of covalent bonding, stereochemistry and aromaticity.
- To study the methods of determining the reaction mechanism.
- To understand the mechanistic aspects of electrophilic and nucleophilic substitution reactions in aliphatic systems.

Unit I: Structure and Bonding

(16 Hours)

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.

Unit II: Basics of Stereochemistry

(16 Hours)

(16 Hours)

Principles of symmetry - Concept of Chirality- Molecular Symmetry and Chirality - 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.

Stereochemistry of molecules with axial chirality-atropisomerism - biphenylsallenes, spiranes and analogues. Helicity and Chirality. Topocity and Prostereoisomerism-Topocity of ligands and faces - Enantiotopic ligands and faces - Diastereotopic ligands and faces. Racemization-methods-Mechanisms of racemization through carbocations, carbanions and freeradicals - Resolution - Methods of resolution.

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 Principle and Curtin-Hammett principle.

Unit III: Aromaticity and Reactive Intermediates

Aromatic character-Huckel's rule and applications-Craig's rule and applications-Consequences of aromaticity - non-alternation in bond length-Resonarce energy from heat of hydrogenation, heat of combustion and Huckel's MO calculation. Alternant and non-alternant hydrocarbonsantiaromtic compounds-paratropic compounds. Aromaticity of azulenes, tropones and annulenes - Structure, stability, generation and reactions of Carbocations (classical and non-classical), carbanions, carbenes, nitrenes and free-radicals.

Unit IV: Methods of Determining Reaction Mechanism (16 Hours)

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: isotope effects: primary, secondary and solvent isotope effect. Correlation Analysis - Linear free energy relationships - Hammett equation

- significance of σ and ρ Applications of Hammett equation-Taft equation and its applications.

UNIT V: Aliphatic Nucleophilic and Electrophilic Substitutions (16 Hours)

Aliphatic Nucleophilic Substitution: $S_N{}^1$ and $S_N{}^2$ 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 reactions-: Von-Braun, Dieckmann, Williamson. Aliphatic Electrophilic Substitution $S_E{}^1$ and $S_E{}^2$ and $S_E{}^i$ mechanisms-effect of substrate structure, leaving group, attacking nucleophile and solvent polarity-Stork-enamine reaction - Haloform reaction.

REFERENCES

- 1. Cahn R S and Derner O C, 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. Finar I L, Organic Chemistry Volume 2, Sixth Edition, ELBS with Longmann, Singapore (1997).
- 5. Eliel E L, Stereochemistry of Carbon Compounds, Tata-McGraw Hill Publishing Company, New Delhi (1998).
- 6. Nasipuri D, Stereochemistry of Carbon Compounds, Second Edition, New-Age International Publishers, New Delhi (1996).
- 7. Clayden Greaves, Warren and Wothers, Organic Chemistry, Oxford University Press, New York (2006).

Sem. I 14PCH1103

Hours/Week: 6 Credits: 5

PHYSICAL CHEMISTRY-I

Objectives

- To understand the concepts and applications of reaction kinetics chemistry.
- To understand the concepts and applications of surface chemistry.
- To understand the electro analytical techniques, instrumentation and applications.

Unit I: Theories of reaction rate

(16 Hours)

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 reactions - Kinetic isotope effect, isokinetic relation and temperature - Theories of unimolecular reactions -Lindemann and RRK -Principle of microscopic reversibility and detailed balancing.

Unit II: Application of ARRT to solution kinetics (16 Hours)

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, and 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 (16 Hours)

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 (16 Hours)

Debye Huckel theory - Radius of ionic atmosphere - Calculations of thickness of ionic atmosphere - Evidences of ionic atmosphere - Asymmetry effect -Electrophoretic effect - Debye Falkenhagen 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 (16 Hours)

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.

REFERENCES

- 1. Laidler K J, Chemical Kinetics, Third edition, New Delhi TATA McGraw Hill Co. (1984).
- 2. Kuriacose and Rajaram, Kinetics and Mechanism of Chemical Transformation, Macmillan & Co, Delhi (1993).
- 3. Huges G, Radation Chemistry, Oxford series (1973).
- 4. Antorpov L, 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. I 14PCH1104

Hours/Week: 4 Credits: 3

ORGANIC CHEMISTRY PRACTICAL-I

Objectives

- To learn the separation of binary organic mixtures.
- To learn the methods of qualitative analysis of organic compounds.
- To learn some single stage preparation of organic compounds.

1. Micro Qualitative Analysis of an organic binary mixture

- i. Pilot separation
- ii. Bulk separation
- iii. Determination of melting and boiling points
- iv. Analysis of organic compounds
- 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-nitro aniline from acetanilide
- iv. Preparation of p-bromo aniline from acetanilide
- v. nitration of methyl benzoate
- vi. m-nitro benzoic acid from m-nitro methyl benzoate.

- 1. Furniss B S, Hannaford A J, Smith P W G and Tatchell A R, Vogel's Textbook of Practical Organic Chemistry- Fifth edition, Pearson publication.
- 2. Vengataswaran V et al., Basic Principle of Practical Chemistry Sultan Chand and sons, New Delhi (1997).
- 3. Ganapragasm and Ramamurthy, Organic Chemistry Lab Manual, Second Edition, S. Vishwanathan Printers and Publishers (P) Ltd., Chennai (2007).
- 4. Organic Chemistry Lab Manual for Micro Qualitative Analysis, Department of Chemistry, St. Joseph's College, Tiruchirappalli. (Private circulation)

Sem. I	Hours/Week: 4
14PCH1105	Credits: 3

PHYSICAL CHEMISTRY PRACTICAL-I

Objectives

- To learn some non-electrical physical chemistry experiments.
- To study the kinetics of some reactions.
- To learn the technique of developing phase diagram of some binary systems.
- To learn the determination methods of physical constants of substances.

Regular 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 $KI + I_2 \leftrightarrow KI_3$.
- 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.

Demonstration experiments

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

REFERENCES

- 1. Venkateswaran V, Veeraswamy R, Kulandaivelu A.R., Basic Principles of Practical Chemistry, (2nd edition), New Delhi, Sultan Chand & sons (1997).
- 2. Daniels et al., Experimental Physical Chemistry, (7th edition), New York, McGraw Hill (1970).
- 3. Findlay A, Practical Physical Chemistry, (7th edition), London, Longman (1959).

Sem. I 14PCH1401

Hours/Week: 4 Credits: 4

IDC-I (WS): INDUSTRIAL PRODUCTS

Objectives

- To learn some of the Industrial products like cement and glass and their manufacturing processes.
- To know the chemistry of dyes, pigments and paints.
- To know about plastics and fibres.
- To learn about fertilizers and fuels.

UNIT I: Cement and Glass

Cement - Composition, types - Portland cement - Composition, types, manufacture (Wet and Dry process), uses - Setting of cement, Glass-Composition, Types, Formation operations - Melting, Blowing, Pressing, Annealing and finishing.

Unit II: Pigments, Dyes and Paints

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

Unit III: Plastics and Fibres

Fibres - Natural and synthetic fibres, Artificial silk, rayon, nylon and Terylene; Plastics - composition, Classification, manufacture, properties and uses.

Unit IV: 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.

Unit V: Cosmetics

Shampoo- composition and its preparation, lipstick -preparation, Face cream and face powder -composition and their preparation. Hair dyes - chemical and herbal dyes. Perfumes and Deodorants.

- 1. Kirk Othmer, Encyclopedia of Chemical Technology.
- 2. Charkarabarthy B N, Industrial Chemistry, Oxford and IBH Prb.Co.
- 3. Sharma B K, Industrial Chemistry, Goel Publishing House.

Hours/Week: 6 Credits: 5

INORGANIC CHEMISTRY - II

Objectives

- To understand the concept of ionic bonding.
- To understand the concept of covalent bonding.
- To learn acids and bases.
- To understand the periodicity of elements and the chemistry of halogens and noble gases.

UNITI: Ionic Bonding

(16 Hours)

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

(16 Hours)

Valence bond theory - resonance - conditions of resonance - formal chargehybridization - 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 BeH₂. VSEPR theory - methane, ethylene - acetylene, ammonia, water, PCl₃F₂ (Bent's rule), SF₄, BrF₃, TeF₅, ICl₂⁻, ICl₄⁻, XeF₂, XeF₄, XeF₆, XeO₃, XeO₄, XeO₂F₂, XeOF₄, phosphorus trihalides, ammonia & NX₃ dipole moments, OF₂ and COF₂. Bond angle - s, p Character relationship - energetics of hybridization.

UNIT III : Acids and Bases

(16 Hours)

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.* NH₃, liq. SO₂, HF and H₂SO₄ as solvents - alkali metals in *liq.* NH₃.

UNITIV: Periodicity and the chemistry of halogens and noble gases (16 Hours)

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 (16 Hours)

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 Structures 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.

- 1. Huheey J E, *Inorganic Chemistry*, (Second Printing) New York, Harper & Row publishers (1972).
- 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).
- 4. Gary L. Miessier & Donald A. Tarr, Inorganic Chemistry (Third Edition), Pearson Education, Singapore (P) Ltd.
- 5. James E. House, Inorganic Chemistry, Elsevier Science and Technbology, 2nd Edition.
- 6. Shiver and Atkin's, inorganic chemistry, W.H. Freeman of Company, 5th Edition.

• To study the mechanistic aspects and synthetic applications of addition and elimination reactions.

substitution reactions of aromatic systems.

Sem. II

14PCH2107

Objectives

• To understand the rearrangement reactions (C-C, C-N, C-O) and their stereochemical aspects.

ORGANIC CHEMISTRY-II

• To learn the mechanistic aspects of electrophilic and nucleophilic

• To understand the various oxidising and reducing reagents and their characteristic reactions.

UNIT I: Aromatic Electrophilic and Nucleophilic Substitutions (16 Hours)

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

Aromatic Nucleophilic Substitution - S_NAr mechanism- S_N^1 (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.

Unit II: Addition Reactions

(16 Hours)

Hours/Week: 6

Credits: 5

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

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

Unit III: Eliminations Reactions

(16 Hours)

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

Unit IV: Oxidation and Reduction Reactions (16 Hours)

Weinberg scheme of redox reactions- Synthetic uses of the following oxidants - DDO, PCC, PDC, Jones reagent and chromyl chloride, MnO₂, SeO₂, KMnO₄, CrO₃, KBrO₃, Thallium nitrate, Pb(OAc)₄, peracids, ozone, periodate, OsO₄, RuO₄ Lemieux-Johnson reagents, Prevost and Woodword reactions, dehydrogenating reagents, Bio-oxidants - catalytic hydrogenation - Synthetic uses of the following reductants: NaNH₂, Wilkinson's catalyst, LAH, NaBH₄, (t-BuO)₃AlH, NaBH₃CN, R₃SnH, Me₃SiCl, alkali metals (Na, Li), Mg-Hg, hvdrazine, MPV reduction, Clemmensen reduction, Wolff-Kishner reduction.

UNIT V: Molecular Rearrangements

(16 Hours)

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

- 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. Gould E S, Mechanism and Structure in Organic Chemistry, Holt-Reinhart and Winston, New York (1959).
- 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).
- 6. Kalsi P S, Stereochemistry: Conformation and Mechanism, 4th Edition, New-Age International Publishers, New Delhi (1997).
- 7. Finar I L, Organic Chemistry Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997).
- 8. Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press, New York (2006).

Hours/Week: 6 Credits: 5

PHYSICAL CHEMISTRY - II

Objectives

- To study the fundamentals and applications of classical mechanics.
- To study the fundamentals and applications of quantum chemistry.
- To understand the symmetry of molecules and its applications.

Unit I: Classical Mechanics

(16 Hours)

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 Schrödinger 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

(16 Hours)

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: Basic Quantum Chemistry

(16 Hours)

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

UNIT IV: Rudiments of Group Theory

(16 Hours)

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

(16 Hours)

Applications of Group theory - Standard reduction formula relating reducible and irreducible representations - Hybridization schemes for atoms in molecules of different geometry - AB₄ tetrahedral, AB₃ triangular planar, AB linear molecules -Symmetries of vibrational modes in non-linear molecules (H₂O, NH₃ and BF₃) - Symmetries of vibrational modes in linear molecules (HCN, CO₂, C₂H₂) -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

- 1. Prasad R K, *Quantum Chemistry*, Ist Edition, New Delhi, Wiley Eastern Ltd, (1992).
- 2. Anderson J M, *Mathematics of Quantum Chemistry*, First Edition, Massachusetts, W. A. Benjamine Inc. (1966)
- 3. Donald A McQuarrie, *Quantum Chemistry*, Indian Edition, Viva Books PrivateLtd.
- 4. Gupta and Kumar, *Classical Mechanics*.
- 5. Chandra A K, *Introductory Quantum Chemistry*, Fourth Edition, Tata McGraw, Hill (1994).
- 6. Levine I N, *Quantum Chemistry*, Fourth Edition, Prentice Hall of India, Pvt. Ltd (1994).
- 7. Atkins PW, Molecular Quantum Mechanics, Clarendon (1973).
- 8. Raman K V, *Group Theory and its Applications to Chemistry*, New Delhi, TATA McGraw Hill Co, (1990).

Hours/Week: 4 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

- i. Determination of saponification value of oil.
- ii. Estimation of iodine value of 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.

REFERENCES

- 1. Furniss BS, Hannaford AJ, Smith PWG, Tatchell AR, *Vogel's Textbook of Practical Organic Chemistry*, Fifth edition, Pearson publication.
- 2. Vengataswaran V et al., *Basic Principle of Practical Chemistry*, Sultan Chand and sons, New Delhi (1997).
- 3. Ganapragasm and Ramamurthy , *Organic Chemistry Lab Manual*, Second Edition, S.Vishwanathan Printers and Publishers (P) Ltd., Chennai (2007).

Sem. II 14PCH2110

Hours/Week: 4 Credits: 3

PHYSICAL CHEMISTRY PRACTICAL-II

Objectives

• To learn some electro analytical experiments.

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 Benzoicacid.
- 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 dibasicacid.
- 8. Conductometric precipitation titration iodide and chloridemixture.
- 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.

Demonstration Experiments

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

- 1. Venkateswaran V, Veeraswamy R., Kulandaivelu A.R., *Basic Principles* of *Practical Chemistry*, Second edition, New Delhi, Sultan Chand & sons, (1997).
- 2. Daniels *et al., Experimental Physical Chemistry*, Seventh edition, New York, McGraw Hill, (1970).
- 3. Findlay A, *Practical Physical Chemistry*, Seventh edition, London, Longman (1959).

Credits: 2

Self Paced Learning: ANALYTICAL CHEMISTRY

Objectives

- To know about the nature of errors and their types
- To know the statistical methods in error analysis
- To know the chromatographic technique its theory, instrumentation, types and applications
- To understand the methods of thermal analysis

UNITI:

ERRORANALYSIS - I

Significant figures- rounding off the values - accuracy and precision- errorsclassification 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.

UNITII:

ERROR ANALYSIS - II

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 III:

CHROMATOGRAPHY-I

Principle of chromatography- retardation factor- classification of chromatographic techniques- partition chromatography: liquid-liquid, paper, gas-liquid chromatography - Adsorption chromatography: Column chromatography- Theory- procedure - applications.

UNITIV:

CHROMATOGRAPHY-II

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.

UNITV:

THERMOANALYTICALMETHODS

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

- 1. Vogel A I, *A Text Book of Quantitative Inorganic Analysis*, Third Edition, London, Longman Group Ltd.
- 2. Day R A and Underwood AL, *Quantitative Analysis*, sixth Edition., PHI (2001).
- 3. Gary A Christian, *Analytical Chemistry*, Sixth Edition, John Wiley & Sons Ltd., (2003).
- 4. Gopalan R, Subramanian P S, Rengarajan K, *Elements of Analytical Chemistry*, Third Edition, Sultan Chand & Sons, New Delhi, (2003).
- 5. Kamboj P C, *University Practical Chemistry*, Vishal Pub., Jalandhar, (2008).
- 6. Dash UN, *Analytical Chemistry Theory and Practice*, Second Edition, Sultan Chand & Sons, New Delhi, (2005).
- 7. Willard and others, *Instrumental Methods of Analysis*, Third edition, East West Press, (1977).

Sem. II 14PSS2401

Hours/Week: 4 Credits: 4

IDC-1: SOFT SKILLS

Objectives

* Introducing learners to the relevant soft skills at the territory level in order to make them gain competitive advantage both professionally and personally.

Module 1: Basics of communication and Effective communication

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

Module II: Resume writing and Interview skills

Resume Writing: What is Resume? Types of Resume? Chronological, Functional and Mixed Resume, Steps in preparation of Resume. Interview Skills: Common interview questions, Attitude, Body Language, The mock interviews, Phone interviews, Behavioral interviews.

Module III: Group discussion and team building

Group Discussion: 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 GDS. Team Building: Team Vs Group - synergy, Stages of Team Formation, the Dabbawala. Leadership - Styles, Work ethics. Personal Effectiveness: Personal Effectiveness: Self Discovery, Self Esteem, and Goal setting. Conflict and Stress Management.

Module IV: Numerical Ability

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, Rations and Proportions.

Module V: Test of reasoning

Verbal Reasoning: Series Completion, Analogy, Data Sufficiency, Assertion and Reasoning, Logical Deduction. Non-Verbal Reasoning: Series, Classification.

References

- 1. Aggarwal, R.S. 2010 Quantitative Aptitude, S. Chand & Sons
- 2 Aggarwal, R.S. 2010. A Modern Approach to Verbal and Non Verbal Reasoning. S.Chand
- 3. Covey, Stephen. 2004. 7 Habits of Highly effective people, Free Press.
- 4. Egan, Gerard. 1994. *The Skilled Helper* (5th Ed). Pacific Grove, Brooks / Cole.
- 5. Khera, Shiv 2003. You Can Win. Macmillan Books, Revised Edition
- 6. Murphy, Raymond. 1998. *Essential English Grammar*. 2nd ed., Cambridge Univ. Press.
- 7. Prasad, L. M. 2000. Organizational Behaviour, S. Chand
- 8. Sankaran, K., & Kumar, M. 2010 *Group Discussion and Public Speaking*. M.I. Pub, Agra, Adams Media.
- 9. Schuller, Robert. (2010). *Positive Attitudes*. Jaico Books.
- 10. Trishna's (2006). *How to do well in GDs & Interviews*, Trishna Knowledge Systems.
- 11. Yate, Martin. (2005). *Hiring the Best: A Manager's Guide to Effective Interviewing and Recruiting*.

Sem. III	
14PCH3112	

Hours/Week: 6 Credits: 5

INORGANIC CHEMISTRY-III

Objectives

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

UNIT I: Theories of Coordination Chemistry (16 Hours)

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 splitting, 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 tetrahedral and square planar complexes.

UNIT II: Basics of Organometallics

(16 Hours)

Types of ligands, hapticty, 16 and 18 electron rules, its applications and limitations. Carbonyls - bonding - terminal, doubly, triply bridged carbonyls - structure of carbonyls - CO stretching frequencies of carbonyls and mixed carbonyls. Carbonyl hydrides - Nitrosyls: terminal, bridging and bent. pi-complexes with olefins- ferrocene and benzenoid metal complexes. Non-benzenoid aromatics as ligands and carbene complexes- fluxional molecules.

UNIIT III: Reaction Kinetics in Coordination Chemistry (16 Hours)

Inert and labile complexes - Stepwise, overall stability constants - Chelate effect - mechanisms - S_N^{1} , S_N^{2} , Solvent intervention, ion pair formation and $S_N^{1}CB$ - 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 (16 Hours)

Types of magnetic behaviour - magnetic susceptibility measurements - Gouy method. Orbital contribution-Spin-orbit coupling and its effects 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 (16 Hours) NMR - Applications of NMR to inorganic compounds - NMR of metal hydrides (¹H NMR), metal carbonyls(¹³C NMR), 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 - FeSO₄, FeCl₃, ferro- and ferricyanide, nitroprusside, Fe₃(CO)₁₂, I₂Br₂Cl₄.

- 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).
- 3. Sutton D, *Electronic Spectra of Transition Metal Complexes*, First Edition, Mc Graw Hill, Australia (1968).
- 4. Basalo F and Pearson R G, *Mechanisms of Inorganic Reactions*, John-Wiley and Sons Inc., New York (1960).
- 5. Kazuo Nakamota, Infrared Spectra of Inorganic and Coordination Compounds, Willey (1970).
- 6. Straughn B P and Walker S, *Spectroscopy* Volumes 1,2 and 3, London, Chapman & Hall, (1976).
- 7. Ebsworth EAV, *Structural Methods in Inorganic Chemistry*, 3rd Ed, Great Britain, ELBS, (1987).
- 8. Drago R S, *Physical Methods in Chemistry*, 3rd Ed., Philadelphia, London, W.B.S. Saunders Company, (1992).
- 9. Gibbs T C, *Principles of Massbauer Specroscopy*, London, Chapman & Hall, (1976).

Sem. III Hours/Week: 6 14PCH3113 Credits: 5 ORGANIC CHEMISTRY - III

Objectives

- To learn the principle, instrumentation and applications of various spectroscopic techniques.
- To learn the basics and applications of synthetic organic chemistry.
- To understand the principle, stereochemistry and applications of photochemistry and Pericyclic reactions.

UNIT I: Organic Spectroscopy - I

(16 Hrs)

UV-Visible spectroscopy-basic principles of electronic transitions-correlation of electronic transitions-instrumental and sample handling techniquesdifferentiating 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 themquantitative studies-inter and intra molecular hydrogen bondingconformational aspects in cyclic 1, 2- and 1, 3- diols - transannular reactions in UV and IR - applications of IR.

UNIT II: Organic Spectroscopy - II

(16 Hrs)

PMR spectroscopy-chemical shift-magnetic non equivalence of protonstypes of coupling and coupling constants (J^1 , J^2 - values) - Karplus equationdeuterium exchange shift reagents-correlation of chemical shift with structure-spin decoupling of exchangeable protons-applications. Fourier Transform. CMR spectroscopy - Basic principles-broad band and offresonance decoupling applications - ESR spectroscopy-applications to organic compounds.

Unit III: Organic Spectroscopy - III

(16 Hrs)

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

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

UNIT IV: Organic Synthetic Methods

(16 Hrs)

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-1,3-diketones- β -keto esters- α -halo ketones. Protecting groups-protection of hydroxyl, carboxyl, carbonyl and amino groups-illustration of protection and deprotection in syntheses.

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

UNIT V: Photochemistry and Pericylic reactions (16 Hrs)

Photochemistry - Fundamental concepts-Joblanskii diagramphotosensitization. Photochemical reactions - photoreduction photooxidation - photochemical rearrangements - Norrish type-I and type -II reactions - Paterno-Buchi reaction - Barton reaction - Ene reaction -Di-*pi* 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.

- 1. March J, *Advanced Organic Chemistry;* Fourth Edition, John-Wiley and Sons, New York (1992).
- 2. Silverstein R M and Bassler G C, *Spectrometric Identification of Organic Compounds, Fourth Edition, John-Wiley and Sons, New York (1993).*
- 3. Kemp W, Organic Spectroscopy, Third Edition, ELBS, London (1987).
- 4. Fleming I, *Spectroscopic Methods in Organic Chemistry*, Fourth Edition, Tata-McGraw Hill Publishing Company, New Delhi (1988).
- 5. Stewart Warren, *Designing Organic synthesis: The Disconnection Approach*, Wiley, New Delhi (1984).
- 6. Clayden, Greaver, Warren and Wothers, *Organic Chemistry*, Oxford University Press, New York (2006).
- 7. Morrision R.T. and Boyd R.N., *Organic Chemistry*, Sixth Edition, Allyn & Bacon Ltd., New York (1976).

Sem. III 14PPS3101

Hours/Week: 6 Credits: 5

Common Core: METHODS OF SPECTROSCOPY AND LASERS

Objectives

- To understand the basic concepts of molecular spectroscopy.
- To study in detail Raman and electronic spectroscopies.
- To study in detail NMR, NQR and ESR spectroscopies.

UNIT-I:

Rotational and Vibrational Spectroscopy

(16 Hours)

Basic aspects of Spectroscopy-characterisation of electromagnetic radiation, quantization of energy. Microwave Spectroscopy-Rotation of molecules and selection rules, Diatomic molecules; Rigid and nonrigid rorator, Rotational constant and centrifugal distortion. Techiniques and instrumentation. Vibrational spectroscopy-diatomic molecules, Harmonic and anharmonic oscillators, zero point energy - force constant - fundamental absorption and overtones (hot bands, fermi resonance)- polyatomic molecules-techniques and instumentation of FTIR.

Unit II:

Raman and NMR spectroscopy

(16 Hours)

-Raman spectroscopy - Raman and Rayleigh scattering - Quantum and classical theories of Raman effect - Pure rotational Raman spectra - Stokes and anti-stokes lines - Vibrational Raman spectra-Mutual exclusion rule - Polarised and depolarized Raman lines - Techniques and instrumentation. NMR - Hydrogen nuclei - Chemical shift and spin - spin splitting - Coupling constant (*J*). Splitting with and without chemical exchange-instrumentation-Interaction between spin and magnetic field - Gyromagnetic ratio - FT NMR.

UNIT III:

ESR spectroscopy

(16 Hours)

ESR-Principle-Position of ESR absorptions - g value - Hyperfine splitting - Zero field splitting - ESR spectrum of free radicals and copper salicyaldehyde complexes.

Moss Bauer spectroscopy -principles of Moss Bauer spectroscopy, Doppler shift, recoil energy, isomer shift, quadrupole splitting- applications to various compounds.

UNITIV:

Electronic Spectroscopy

(16 Hours)

Electronic spectra - Electronic spectra of diatomic molecules - Born -Oppenheimer approximation- vibrational coarse structure- Franck - Condon Principle-, Dissociation energy and dissociation products - rotational fine structure of electronic vibration -vibration transition - Fortrate Diagram. Electronic angular momentum in diatomic molecules-spectrum of Molecular hydrogen - Molecular photoelectron spectroscopy - UV photo electron spectroscopy and X-ray photo electron spectroscopy.

UNIT V:

Laser devices and their Applications

(16 Hours)

Principle - pumping He-Ne laser Carbon di oxide laser, semi conductor laserholography recording and reconstruction-applications laser induced fusionfusion process- stimulated Raman scattering laser in isotope separation lidar-laser tracking- lasers in industry and medicine.

- 1. Banwell C N, *Molecular spectroscopy*, New Delhi, TATA McGraw Hill Co. (1997).
- 2. Drago R S, *Physical Methods in Inorganic Chemistr*, 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 Volume 1,2,3*, New York, London Chapman and Hall, A Halstet Press Book, John Wiley & Sons Ins. (1975).
- 5. Barrow G M, *Introduction to Molecular Spectroscopy*, Tata McGraw-Hill Edition (1993).
- 6. Gurdeep R Chatwal and Sham K Anand, *Spectroscopy*, Himalaya Publishing House (2009).

Sem. IIIHours/Week: 414PCH3114Credits: 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.

REFERENCES

- 1. Shevla G, *Vogel's Inorganic qualitative Analysis*, Seventh edition, Prentice Hall (1996).
- 2. Ramanujam V, *Inorganic Semi-micro Qualitative Analysis*, Third Edition, National Publishing Company, Chennai (1990).

Sem. III 14PCH3201A

Hours/Week: 4 Credits: 4

Core Elective-1A: THERMODYNAMICS-I

Objectives

- To understand the fundamental and applications of statistical thermodynamics.
- To understand the fundamental and applications of partial molar properties.
- To study the basics and applications of chemical thermodynamics.
- To study the instrumental techniques used in chemical thermodynamics.

UNIT I: Fundamentals of Statistical Thermodynamics(12 Hrs)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-Phase space-Thermodynamic probability-Statistical equilibrium-. Maxwell--Boltzmann statistics -Derivation of M.B. statistics-Relationship between entropy and probability-Statistical meaning of third law of thermodynamics.

UNIT II: Applications of Statistical Thermodynamics (12 Hrs)

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 *Cp*, *Cv* using partition function-Sackur-Tetrode equation-Quantum statistics. Bose Einstein statistics- -Fermi Dirac statistics-. Electronic heat capacity of gases-Nulear spin statistics-Statistical basis of entropy of hydrogen gas, ortho and para nuclear states, nuclear spin entropy.

UNIT III: Chemical Thermodynamics I

(12 Hrs)

Partial molar properties - 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 - 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).

UNITIV: Chemical Thermodynamics II and Numerical Problems in Thermodynamics (12 Hrs)

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.

Simple Numerical calculations on I law and II law of thermodynamics based on 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.

UNIT V: Chemical Thermodynamics III

(12 Hrs)

Joule Thomson effect. III law of thermodynamics - Thermochemistry - Kirchoff's equation.

Determination of ΔH by Bomb Calorimeter - Determination of volume of mixing by relative density method.

REFERENCES

- 1. Kuriakose J.C and Rajaram J.C, *Thermodynamics*, Jalandar Shoban Lal Co., (1996).
- 2. Gupta M.C, *Statistical Thermodynamics*, Wiley-Eastern Limited, Madras (1997).
- 3. Glasstone S, *Thermodynamics for Chemists*, New Delhi, East West Affiliated Pvt. Ltd, (1969).
- 4. Donald McQuarrie, *Stastistical Thermodynamics*, Indian Edition, Viva Books Private Ltd., New Delhi (2003).
- 5. Ferrell L Hill, *Introduction to Statistical Thermodynamics*, Addison-Wesley Publishing Company, INC, London (1962).

Sem. III 14PCH3201B

Hours/Week: 4 Credits: 4

Core Elective-1B: THERMODYNAMICS-II

Objectives

- To study the basics and applications of chemical thermodynamics.
- To understand the basics and applications of non- equilibrium thermodynamics.
- To understand the basics and applications of phase equilibria.
- To study the instrumental techniques used in chemical thermodynamics.

UNITI

(12 Hrs)

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.

UNITII

(12 Hrs)

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 $L_{12}=L_{21}$).

UNITIII

(12 Hrs)

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 IV

(12 Hrs)

Phase equilibrium - phase rule - one, two and three component systems -Water, sulphur, carbon dioxide, lead - silver, KI - water, benzene - naphthalene, ferric chloride - water and acetic acid - chloroform - water.

UNIT V (12 Hrs)

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.

REFERENCES

- 1. Kuriakose J C and Rajaram J C, *Thermodynamics*, Jalandar Shoban Lal Co., (1996).
- 2. Glasstone S, *Thermodynamics for Chemists*, New Delhi, East West Affiliated Pvt. Ltd, (1969).
- 3. Lewis G N and Randall M, *Thermodynamics*, Second Reprint, McGraw-Hill Book Company (1961).
- 4. Ira N. Levine, *Physical Chemistry*, Fifth edition, Tata Mc Graw-Hill Publication company Ltd., New Delhi (2002).
- 5. Donald Mc Quarrie, *Stastistical Thermodynamics*, Indian Edition, Viva Books Private Ltd., New Delhi (2003).
- 6. Ferrell L Hill, *Introduction to Statistical Thermodynamics*, Addison-Wesley Publishing Company, INC, London (1962).

Sem. III 14PCH3402

Hours/Week: 4 Credits: 4

IDC (III) (BS): 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 (12 Hours)

Definition: Food, Food Pyramid - Health-Hygiene- mal-, under- and overnutrition, their causes and remedies, sanitation, Carbohydrates -Classification, Biological functions, Protein- Classification, Biological functions, Vitamins - Classification, Biological functions.

UNIT II:

Drugs (12 Hours)

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

Unit III:

Body fluids

(12 Hours)

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

Unit IV:

Enzymes, Hormones, Digestion

(12 Hours)

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

(12 Hours)

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 14PCH4115

Hours/Week: 4 Credits: 4

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.

UNITI:

Solid State -I

(12 Hours)

Elements of crystallography - space lattices-unit cell-crystal systems - Xray 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 ReO₃ structure.

UNIT II :

Solid State -II

(12 Hours)

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 - nonstoichiometric defects - n, p semiconductors - structure of solids- free electron and band theory of solids. Electrical conductivity and superconductivity high temperature superconductors.

UNIT III :

Photochemistry

(12 Hours)

Laws of photochemistry - Photo physical processes - Jablonski diagram -Fluorescence - Phosphorescence - Kasha's rule - Stoke's shift - Types of electronic transitions in transition metal complexes - *Photo chemistry of transition metal complexes* - Photo substitution - Photo aquation - Adamson's rules -Photo rearrangement - Photo redox reations. *Photo chemistry of organo metallic compounds*.

Unit IV :

Bio-inorganic Chemistry -I

(12 Hours)

Structure and function of chlorophyll - Role of Mg^{2+} ion- Structure and function of Haemoglobin - Cooperative effect in Haemoglobin - Role of Globin - Structure and function of Myoglobin - Structure and function of Cytochrome C.

UNIT V:

Bio-inorganic Chemistry-II

(12 Hours)

Structure and function of Blue copper proteins - Structure and function of Vitamin B₁₂- Invivo nitrogen fixaction- Fe-S protiens- Ionophores - Ion transport mechanism in cell membrane - Na-K pump. Role of metal ions in DNA replication, Transcription, Translation - Role of cis platin in the treatment of cancer.

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 HV, 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. Lipard S J and Berg JM, *Principles of Bioinorganic Chemistry*, Panima Publishing Corporation, (2005).
- 11. Rohatgi-Mukherjee K K, *Fundamentals of Photochemistry*, New Age International Publishers, New Delhi, (2006).
- 12. K. Hussain Reddy, *Bioinorganic Chemistry*, New Age international publishers, (2007).

Sem. IV 14PCH4116

Hours/Week: 4 Credits: 4

ORGANIC CHEMISTRY-IV

Objectives

- To study the 12 principles of Green chemistry and its application in synthesis.
- To learn the basics and application of organometallics and electro-organic methods in organic synthesis.
- To understand the stereochemistry aspects- asymmetric synthesis and stereoselective reactions.
- To know the fundamentals of electroorganic synthesis.

Unit I:

Green Chemistry

(12 Hrs)

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

Unit II:

Organometallics in Organic Synthesis

(12 Hrs)

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 - Synthetic applications of organozinc, organocadmium reagents.

Chan-Lam Coupling, Hiyama coupling - Corey-Fuchs Reaction, Me₂CuLi (Gillman's reagent), Heck reaction, Suzuki coupling, Stille coupling, Sonogashira reaction, Fukuyama Coupling - Negishi Coupling, Kumada Coupling. Paulson-Khand reaction, Vollhart co-trimerization.

Unit III:

Asymmetric Synthesis and Name Reactions

(12 Hrs)

Nucleophilic addition to 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 - Alkylation reactions - C versus O alkylation - enamines and selective alkylation. Uses of special reagents containing B, P and Si. Baylis-Hillman reaction - Biginelli reaction - Mukaiyama aldol reaction - Prins reaction, Mitsunobu reaction - Weinreb ketone synthesis Henry reaction - Hosomi-Sakurai reaction.

Unit IV:

Stereoselective Reactions in Cyclic Compounds

(12 Hrs)

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 V:

Electro Organic Chemistry

(12 Hrs)

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.

REFERENCES

- 1. March J, *Advanced Organic Chemistry;* Fourth Edition, John-Wiley and Sons, New York (1992).
- 2. Paula yurkanis Bruice, *Organic Chemistry*, Seventh Edition, Prentice Hall (2013).
- 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*, 1st Edi., Oxford University Press, UK, (2001).
- 5. Paul T Anastas, Text Book on Green Chemistry, OUP, (2006).
- 6. 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).
- 7. Paul T Anastas and John C Warner, Green Chemistry: Theory and Practice, Oxford University Press, UK (1998).

Sem. IV 14PCH4117

Hours/Week: 4 Credits: 4

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.
- To know the characterization methods of complexes

Experiments

- 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. Quantitative analysis of a mixture of copper(volumetric) and zinc (gravimetry)
- 5. Preparation of any three complexes
- 6. Determination of meff of a complex by Gouy method (internal evaluation only)
- 7. IR interpretation of a complex to find out the mode of coordination (internal evaluation only)
- 8. Interpretation of electronic spectrum of a complex (internal evaluation only)

- 1. Vogel A I, A Text Book of Quantitative Inorganic Analysis, Third Edition., London, Longman Group Ltd.
- 2. Department material, St. Joseph' College (Autonomous), Tiruchirappalli.

Sem. IV 14PCH4202A

Hours/Week: 4 Credits: 4

Core Elective-IIA: PHYSICAL CHEMISTRY-III

Objectives

- To know the importance of emf measurement
- To study the various electro analytical techniques, instrumentation and applications.
- To understand the concepts and applications of quantum chemistry.

Unit I:

EMF Measurements and Applications

(12 Hours)

EMF and thermodynamics quantities - Nernst equation - Gibb's Helmoltz relation and EMF - Reversible electrodes - Types- electrode potentials - single electrode potential - electrochemical series - chemical cells - concentration cells with ant without transference- Applications of EMF measurements - Activity coefficients and solubility determination- Storage and Fuel cells.

Unit II:

Electro analytical Techniques - I

(12 Hours)

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 Zn²⁺ and Cd²⁺)-Cyclic voltametry, Principle, Experimental set up - Cyclic voltammogram of Fe²⁺ in H₂SO₄ - Anodic peak current - Cathodic peak current - Electrochemically reversible couple - Cathodic peak potential - Electrochemically irreversible couple - Outline of applications.

UNIT III:

Electro analytical Techniques II

(12 Hours)

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).

UNITIV:

Applications of Quantum Chemistry-I

(12 Hours)

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.

UNITV:

Applications of Quantum Chemistry-II

(12 Hours)

The Born - Oppenheimer approximation - VB theory of hydrogen molecule and MO theory of molecular ion (H^{2+}) - coulomb integral, exchange integral and overlap integral. Construction of sp, sp² and sp³ hybrid orbitals - Huckel molecular orbital theory - principles and applications to ethylene, butadiene and benzene. Huckel calculation of pi-electron energies.

- 1. Vogel A I, Text book of Quantitative Inorganic Analysis ELBS (1978).
- 2. Donald A McQuarrie, *Quantum Chemistry*, Indian Edition, Viva Books Private Limited (2005).
- 3. Noel M and Vasu K I, *Cyclic voltammetry and the Frontiers of Electrochemistry*, Oxford and IBH (1990).
- 4. Kissinger PT and Heinman, *Laboratory Techniques in Electroanalytical Chemistry*, Editors, Marcel Dekker, Inc., New York (1984).
- 5. Willard, Merit, Dean and Settle, *Instrumental Methods of Analysis*, CBS Publication (1986).
- 6. Anatharaman R, *Fundamentals of Quantum Chemistry*, McMillan, New Delhi (2001).
- 7. Prasad R K, Quantum Chemistry, Wiley Eastern Ltd, New Delhi (1992).
- 8. Chandra A K, *Introduction to Quantum Chemistry*, Tata-MaGraw Hill, New Delhi (1997).

Sem. IV 14PCH4202B

Hours/Week: 4 Credits: 4

Core Elective-IIB: POLYMER CHEMISTRY

Objectives

- To understand the basic concepts of polymer chemistry.
- To study the stereochemical, morphological and other properties of polymers
- To study in detail the applications and kinetics of polymerization techniques.

Unit 1:

Introduction to Polymer Science

(12 Hrs)

Polymer science-History - Concepts and terminology. Classification of polymers (with suitable examples) based on origin, structure, backbone, branching, action of heat, ultimate form and use, crystalline and amorphous behaviour Ladder, semi-ladder and spiro polymers.

Molecular forces in polymers - dipole forces, induction forces, dispersion forces, H-bond. Dependence of physical properties on intermolecular forces. Monomers, structure and main features of some common polymers and polyurethane elastomers.

Inorganic polymers: Types of inorganic polymers, preparation, structure and properties of polyphosphazenes, polysiloxanes, polysilanes, polygermanes and polystannanes.

Unit 2:

Stereochemistry and Conformation of Polymers

(12 Hrs)

Constitutional isomerism-positional isomerism and branching, substitutional isomerism (with suitable examples). Configuration and conformation of macromolecules: stereoisomerism-optical isomerism and geometrical isomerism, configuration of polymer chains-stereoregular polymers, tacticity in polymers-monotactic and ditactic polymers.

Experimental and spectroscopic methods for the determination of configuration, conformation of single macromolecule, conformation in the crystal, micro conformation in solution, ideal coil molecules in solution, compact molecules. Optically active poly(olefins), poly(amino acids), proteins. Conformational transitions.

Unit 3:

Morphology and Order in Crystalline Polymers

Polymer morphology: common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallizability-mechanism of crystallization Polymer single crystals: lamellar structure of polymers-fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

Structure of polymers: crystallized from melt-super crystalline structures, spherulitic morphology, mechanism of spherulite formation. Theories of crystallization, kinetics- Avrami equation, Hoffman's nucleation theory, the entropic barrier theory. Strain induced morphology, cold drawing, morphology changes during orientation. Theory and application of XRD, SEM and DSC in determining the crystallinity of polymers.

Unit 4:

Polymer Solutions

(12 Hrs)

(12 Hrs)

Solubility of low molecular weight substances and polymers. Theories of polymer solubility, different stages of polymer solubility, non solvents, solubility of amorphous and crystalline polymers, solubility parameter concept. Thermodynamics of polymer solution:lattice theory-advantages and limitations of lattice theory,Flory-Huggins and Flory-Krigbaum theories -advantages and limitation of FH and FK theories, corresponding state theories, Flory temperature, polymer - solvent interaction parameter, the unperturbed polymer chain, expansibility factor, entropy,enthalpy and free energy of mixing of polymer solution, phase separation in polymer systems. The models of De Gennes and Edwards tube model (worm model), self avoiding random walk, scaling concepts in polymer systems, pearl model.

UNITV:

Kinetics of Polymer Chemistry

(12 Hrs)

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.

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REFERENCES

- 1. Gowariker V R, Viswanathan N V, Sreedhar J, *Polymer Science*, New Age International (2011).
- 2. Billmeyer F W Jr., *Text book of Polymer Science*, Third Edition, John Wiley & Sons (1984).
- 2. Sperling LH, *Introduction to Physical Polymer Science*, Fourth Edition, Wiley-Inter science (2005).
- 4. Cowie JMG, Arrighi V, *Polymers: Chemistry and Physics of Modern Materials*, Third Edition, CRS Press (2007).
- 5. Bower DI, *An Introduction to Polymer Physics*, Cambridge University Press (2002).
- 6. Chanda M, Introduction to Polymer Science and Chemistry, A Problem Solving Approach, CRS Press (2006).
- 7. Flory PJ, *Principles of Polymer Chemistry*, Cornell University Press(1953).
- 8. de Gennes PG, *Scaling Concepts in Polymer Physics*, Cornell University Press (1979).
- 9. Teraoka, *Polymer Solutions: An Introduction to Physical Properties*, John Wiley & Sons, (2002).
- 10. Chandrasekhar V, *Inorganic and Organometallic Polymers*, Springer (2005).

Sem. IV 14PCH4203A

Hours/Week: 4 Credits: 4

Core Elective-IIIA: NATURAL PRODUCTS

Objectives

- To understand the structure, reactions and biological functions of biomolecules.
- To learn the preparation, reactions of the five, six and fused heterocyclics.
- To study the nature, structure, isolation, classification, functions and structural elucidation of natural products.

UNIT I:

Carbohydrates

(12 Hours)

Carbohydrates- Ring structures-Structural Determination of D(+)-glucose only. Citric acid cycle- Structure of fructose, sucrose, maltose, lactose and cellobiose-. Structural difference between starch and cellulose.

UNIT II:

Proteins & Nucleic acids

(12 Hours)

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:

Alkaloids, Terpenoids and Antibiotics

(12 Hours)

Alkaloids: Introduction-extraction-classification- structural elucidation of papaverine only.

Terpenoids: Introduction-extraction-classification- structural elucidation of Zingiberene only.

Antibiotics: structure - Activity - Relationship of chloramphenicol - structure and functions of penicillin, streptomycin and terramycin.

UNITIV:

Hormones

(12 Hours)

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

UNITV:

Heterocyclics

(12 Hours)

Preparation, physical properties and reactions of 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).

Reference

- 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. IV 14PCH4203B

Hours/Week: 4 Credits: 4

Core Elective-IIIB: PHARMACEUTICAL CHEMISTRY

Objectives

- To study the design, structure and structure activity relationship of drugs.
- To understand the various modes of spread of common diseases and their treatment.
- To learn the advanced drugs for new diseases.

Unit-I: Introduction to Chemistry of Drugs (12 Hours)

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- Colorantsm Flavoring agents - Sweeteners - Stabilizers- suspending agents- Ointment bases- Solvents.

Unit-III: Common Diseases and Treatment (12 Hours)

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- treatmentdiseases 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

(12 Hours)

(12 Hours)

(12 Hours)

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).

Hours/Week: 10 Credits: 5

DISSERTATION & VIVA VOCE