

M.Sc. Chemistry

Curriculum and Syllabus (Based on Choice based credit system) Effective from the Academic Year 2018 – 2019

Department of Chemistry School of Basic Sciences

PROGRAM EDUCATIONAL OBJECTIVES(PEO)

- PEO 1 Postgraduate will have significant opportunities in various service domains at National and International level, and can work as scientist, analyst, quality controller, academics, research organizations and set chemical testing labs.
- PEO 2 On the basis of specialized knowledge and experience, postgraduate students will be able to do synthesis, separation, analysis, computational design and development of new products.
- PEO 3 Post-graduate have leadership quality to handle all kind of circumstances in diversities by providing interdisciplinary and multidisciplinary learning environment.
- PEO 4 To encourage leadership qualities in graduates with strong communication skills, mold them as good team players and managers so that they have the competence to function effectively in multi disciplinary orientation teams.
- PEO 5 Postgraduate will be able to formulate, investigate and analyze scientifically real life problems along with ethical attitude which works in multidisciplinary team

PROGRAM OUTCOME

- PO1 **Problem analyze:** Identify, formulate, review research literature and analyze the chemical problems reaching substantiated conclusions using basics concepts of mathematics, physics and biology.
- PO2 **Design and development of solutions:** Design solutions for complex chemical problems and design systems, components or processes that meet specified needs with appropriate consideration for public health and safety, cultural, societal, and environmental considerations.
- PO3 **Conduct investigations of complex problems:** Use research based knowledge and including design of experiments, analysis and interpretation of data, and synthesis of information to provide valid conclusions.

PROGRAM SPECIFIC OUTCOME (PSO)

- PSO1 To Job opportunities in wide sector of Chemical & Allied industries
- PSO2 Competent to take challenging positions in industry, academics and government sectors by learning various analytical techniques such as UV, IR, NMR, Chromatography etc and their applications.
- PSO3 To execute new ideas in the field of research and to develop principles and techniques of science through seminars and the project.

BOARD OF STUDIES

S. No	NAME	AFFILIATION	ROLE
1.	Dr . G.Nithya	Associate Professor & HoD, Department of Chemistry, Vels Institute of Science, Technology and Advanced Studies, Pallavaram, Chennai - 600 117.	Chair Person
2.	Dr. Narasimhan Srinivasan	Chairman and Managing Director,Asthagiri Herbal Research Foundation,Perungudi.	
3.	Mr.V. Neelakantan	Managing Director,External ExpertKousikh Therapeutics Private Limited,External ExpertGerugambakkamExternal Expert	
4.	Ms. M. Vidhya lakshmi	Chemist, Instrumentation department, ABC Techno labs India Private Limited. Alumini Member	
5.	Dr. R. A. Kalaivani	Professor & Director, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram,Chennai - 600 117.	Internal member
6.	Dr. T. Somanathan	Associate Professor, Department of Chemistry, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram,Chennai - 600 117.	Internal member
7.	Dr.M. Revathy	Associate Professor, Department of Chemistry, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram,Chennai - 600 117.	Internal member
8.	Mr.V.Sriraman	Assistant Professor, Department of Chemistry, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram,Chennai - 600 117.	Internal member
9.	Dr.R.Sudha	Assistant Professor, Department of Chemistry, School of Basic Sciences, Vels Institute of Science, Technology and Advanced Studies, Pallavaram,Chennai - 600 117.	Internal member

VELS INSTITUTE OF SCIENCE, TECHNOLOGY AND ADVANCED STUDIES (VISTAS)

CHENNAI - 600 117

REGULATIONS 2018

CHOICE BASED CREDIT SYSTEM

DEGREE OF MASTER OF SCIENCE IN CHEMISTRY

1. DURATION OF THE PROGRAMME

1.1. Two years (four semesters)

1.2. Each academic year shall be divided into two semesters. The odd semesters shall consist of the period from July to November of each year and the even semesters from January to May of each year.

1.3 There shall be not less than 90 working days for each semester.

2. ELIGIBILITY FOR ADMISSION

2.1. Candidates for admission to the first year of the degree of Master of Science courses shall be required to have passed the undergraduate Examinations in chemistry conducted by the Government of Tamil Nadu or an Examination accepted as equivalent thereof by the Syndicate of the Vels Institute of Science, Technology & Advanced studies.

3. CREDIT REQUIRMENTS AND ELIGIBILITY FOR AWARD OF DEGREE

3.1. A Candidate shall be eligible for the award of the Degree only if he/she has undergone the prescribed course of study in a College affiliated to the University for a period of not less than two academic years and passed the examinations of all the four Semesters prescribed earning a minimum of 90 credits and also fulfilled such other conditions as have been prescribed thereof.

4. COURSE OF STUDY, CREDITS AND SCHEME OF EXAMINATION

4.1. The Course Components and Credit Distribution shall consist

(Minimum number of Credits to be obtained)

Credit Assignment Each course is assigned certain number of credits based on the following: Contact period per week CREDITS

- 1 Lecture Period 1 Credit
- 1 Tutorial Period 1 Credit

2 Practical Periods - 1 Credit

(Laboratory / Seminar / Project Work / etc.)

5. REQUIREMENTS FOR PROCEEDING TO SUBSEQUENT SEMESTER

5.1. **Eligibility:** Students shall be eligible to go to subsequent semester only if they earn sufficient attendance as prescribed thereof by the Board of Management from time to time.

5.2. **Attendance:** All Students must earn 75% and above of attendance for appearing for the University Examination. (Theory/Practical)

5.3. **Condonation of shortage of attendance:** If a Student fails to earn the minimum attendance (Percentage stipulated), the HODs shall condone the shortage of attendance up to a maximum limit of 10% (i.e. between 65% and above and less than 75%) after collecting the prescribed fee towards the condonation of shortage of attendance. Such fees collected and should be remitted to the University.

5.4. Non-eligibility for condonation of shortage of attendance: Students who have secured less than 65 % but more than 50 % of attendance are NOT ELIGIBLE for condonation of shortage of attendance and such Students will not be permitted to appear for the regular examination, but will be allowed to proceed to the next year/next semester of the program

5.5. **Detained students for want of attendance:** Students who have earned less than 50% of attendance shall be permitted to proceed to the next semester and to complete the Program of study. Such Students shall have to repeat the semester, which they have missed by rejoining

after completion of final semester of the course, by paying the fee for the break of study as prescribed by the University from time to time.

5.6. **Condonation of shortage of attendance for married women students:** In respect of married women students undergoing UG programs, the minimum attendance for condonation (Theory/Practical) shall be relaxed and prescribed as 55% instead of 65% if they conceive during their academic career. Medical certificate from the Doctor together with the

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attendance details shall be forwarded to the university to consider the condonation of attendance mentioning the category.

5.7. **Zero Percent (0%) Attendance:** The Students, who have earned 0% of attendance, have to repeat the program (by rejoining) without proceeding to succeeding semester and they have to obtain prior permission from the University immediately to rejoin the program.

5.8. **Transfer of Students and Credits:** The strength of the credits system is that it permits inter Institutional transfer of students. By providing mobility, it enables individual students to develop their capabilities fully by permitting them to move from one Institution to another in accordance with their aptitude and abilities.

5.8.1. Transfer of Students is permitted from one Institution to another Institution for the same program with same nomenclature. Provided, there is a vacancy in the respective program of Study in the Institution where the transfer is requested. Provided the Student should have passed all the courses in the Institution from where the transfer is requested.

5.8.2. The marks obtained in the courses will be converted and grades will be assigned as per the University norms.

5.8.3. The transfer students are not eligible for classification.

5.8.4. The transfer students are not eligible for Ranking, Prizes and Medals.

5.8.5. Students who want to go to foreign Universities upto two semesters or Project Work with the prior approval of the Departmental / College Committee are allowed to get transfer of credits and marks which will be converted into Grades as per the University norms and are eligible to get CGPA and Classification; they are not eligible for Ranking, Prizes and Medals.

6. EXAMINATION AND EVALUATION

6.1. Register for all subjects: Students shall be permitted to proceed from the First Semester up to Final Semester irrespective of their failure in any of the Semester Examination. For this purpose, Students shall register for all the arrear subjects of earlier semesters along with the current (subsequent) Semester Subjects.

6.2. Marks for Internal and End Semester Examinations.

6.2.1 There shall be no passing minimum for Internal.

6.2.2 For external examination, passing minimum shall be 50% [Fifty Percentage] of the maximum marks prescribed for the paper for each Paper/Practical/Project and Viva-Voce.

6.2.3 In the aggregate [External/Internal] the passing minimum shall be of 50%.

6.2.4. He / She shall be declared to have passed the whole examination, if he/she passes in all the papers and practical wherever prescribed as per the scheme of the examinations by earning 90 CREDITS.

7. MAXIMUM PERIOD FOR COMPLETION OF THE PROGRAMS TO QUALIFY FOR A DEGREE

7.1. A Student who for whatever reasons is not able to complete the programs within the normal period (N) or the Minimum duration prescribed for the programme, may be allowed two years period beyond the normal period to clear the backlog to be qualified for the degree. (Time Span = N + 2 years for the completion of programme)

8. REVISION OF REGULATIONS, CURRICULUM AND SYLLABI

The University may from time to time revise, amend or change the Regulations, Curriculum, Syllabus and Scheme of examinations through the Academic Council with the approval of the Board of Management.

M.Sc. CHEMISTRY CURRICULUM

Total number of Credits: 90

	Code	Course	Hour/Week			
Category			Lecture	Tutorial	Practical	Credits
SEMESTER	-1		1			
CORE	18CMSG11	Organic Chemistry-I	4	0	0	4
CORE	18CMSG12	Inorganic Chemistry – I	4	0	0	4
CORE	18CMSG13	Physical Chemistry-I	4	0	0	4
DSE		Discipline Specific Elective- I	3	0	0	3
DSE		Discipline Specific Elective- II	3	0	0	3
GE		Generic Elective-I	1	0	2	2
CORE	18PMSG11	Physical Chemistry - Practical I	0	0	6	3
			19	0	8	23
SEMESTER	- 11	· ·		·	-	•
CORE	18CMSG21	Organic Chemistry – II	4	0	0	4
CORE	18CMSG22	Inorganic Chemistry – II	4	0	0	4
CORE	18CMSG23	Physical Chemistry – II	4	0	0	4
DSE		Discipline Specific Elective- III	3	0	0	3
CORE	18PMSG21	Organic Chemistry - Practical II	0	0	6	3
CORE	18PMSG22	Analytical Chemistry - Practical III	0	0	6	3
CORE	18IMSG21	Internship	0	0	30	2
			15	0	42	23
SEMESTER		1	I			1
CORE	18CMSG31	Organic Chemistry –III	4	0	0	4
CORE	18CMSG32	Inorganic Chemistry – III	4	0	0	4
CORE	18CMSG33	Physical Chemistry-III	4	0	0	4
DSE		Discipline Specific Elective-IV	3	0	0	3
DSE		Discipline Specific Elective- V	3	0	0	3
GE		Generic Elective-II	2	0	0	2
CORE	18PMSG31	Inorganic Chemistry - Practical IV	0	0	6	3
			20	0	6	23
SEMESTER				1		T
CORE	18CMSG41	Electro analytical and Separation Techniques	5	0	0	5
DSE		Discipline Specific Elective –VI	4	0	0	4
CORE	18RMSG41	Project work	0	0	24	12
			9	0	24	21
		Total	63	0	80	90

LIST OF DISCIPLINE SPECIFIC ELECTIVE COURSES

S.No.	Subject Code	Subject Title
		Macromolecular Chemistry
		Analytical Techniques
		Separation Techniques
		Natural products
		Pharmaceutical Chemistry
		Nuclear and photochemistry
		Chemical & Instrumental Methods of Drug Analysis
		Synthesis of active Pharmaceutical ingredients and their manufacture
		Organometallic Chemistry and Photochemistry
		Organic Spectroscopy
		Stereochemistry and Reaction Mechanism
		Novel materials and green industrial catalysis
		Electrochemistry and Group Theory
		Inorganic Chemistry
		Fundamentals of Biochemistry
		Organic name reactions and synthesis of reagents
		Pharmaceutical Formulation Technology
		Enzyme technology and their entrepreneurial skills
		Synthetic Organic Chemistry
		Strategic Management of Pharma Industry.

LIST OF GENERIC ELECTIVE COURSES

S.No.	Subject Code	Subject Title
		Soft skill – I
		Soft skill – II
		Green Chemistry
		Cheminformatics
		Food Chemistry and Adulteration

Syllabus Core Courses

ORGANIC CHEMISTRY – I

Course Objective:

- > To learn the salient features of optical activity and geometrical isomers of organic compounds.
- > To study the mechanism of substitution reactions in aliphatic and aromatic systems.

UNIT-I Stereochemistry

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Optical activity and chirality. Classification of chiral molecules as asymmetric and dissymmetric. Identification of enantiotopic, homotopic, diastereotopic hydrogens and prochiral carbons in compounds containing up to ten carbons only. Stereospecific and stereo selective reactions. A brief study of dissymmetry of allenes, spiranes ,biphenyl compounds. Absolute configuration-R,S notation of biphenyls and allenes. Fischer projection. Inter conversion of Sawhorse, Newman and Fischer projections. Molecules with more than one asymmetric center (restricted to five carbons) Eg. Erythro and threo compounds. Asymmetric synthesis. Crams's rule. Geometrical isomerism. E,Z nomenclature of olefins. Geometrical and optical isomerism (if shown) of disubstituted cyclopropane, cyclobutane and cyclopentanes.

UNIT-II Aliphatic Nucleophilic Substitution reactions

 S_N^1 , S_N^2 and S_N^1 mechanisms –Neighbouring group participation –reactivity, structural and solvent effects- substitution in norbornyl and bridgehead systems –substitution at allylic and vinylic carbons substitution by ambident nucleophiles-substitution at carbon doubly bonded to oxygen and nitrogen-alkylation and acylation of amines, halogen exchange. Von-Braun reaction, alkylation and acylation of active methylene carbon compounds, hydrolysis of esters, Claisen and Dieckmann condensations.

UNIT-III Aromatic Substitution Reaction – II

Nucleophilic substitutions-Method for the generation of benzyne intermediate and reactions of aryne intermediate-Nucleophilic substitution involving diazonium ions. Aromatic Nucleophilic substitutions of activated halides. Ziegler alkylation. Chichibabin reaction.

UNIT-IV Aromaticity

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

UNIT-V Aromatic Substitution Reaction–I

Electrophilic Substitutions-The arenium ion mechanism –Orientation and reactivity (ortho, meta and para directing groups), Hammett equations. Typical reactions – nitration, halogenation, alkylation, acylation and diazonium coupling. Formylation reactions-Gatterman, Gatterman-Koch, Vilsmeyer-Hack and Reimer –Tieman reaction. Electrophilic substitution of furan, pyrrole, thiophene, pyridine and pyridine -N-oxide.

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Outcomes:

- To learn the concept stereochemistry and its importance
- To know what is aliphatic nucleophilic substitution
- To understand the various types of aliphatic nucleophilic substitution
- To learn what is aromatic substitution reaction
- To familiarize the various types of aromatic substitution reaction and their Mechanism

TEXT BOOKS:

- 1. R.O.C. Norman, Organic Synthesis, Chapman and Hall, New York, 2nd edition, 1980.
- S.M. Mukherji, S.P. Singh, Organic Reaction Mechanism, MacMillan India Ltd., Chennai, 1990.
- 3. Francis A. Carey, Richard J. Sunderg, Advanced Organic Chemistry Part A and B, Plenum Press, 3rd Edition, 1990.

- 1. Jerry March, Advanced Organic Chemistry, Wiley Eastern Limited, Fourth edition, New Delhi, 1999.
- 2. John Mc. Murray, Organic Chemistry, Cengage Learning, 8th edition, 2011.
- 3. T.L. Gilchrish and C.W. Rees, Carbenes, Nitrenes and Arynes ,Thomas Nelson and Sons Ltd., London, 1969.

INORGANIC CHEMISTRY – I

Course Objective:

- Structural study of poly acid, Inorganic polymers and Boron hydrides .
- To learn about the complexes with respect to stability, stereoisomerism, the nature of bonding, electron transfer reactions and substitution reaction in square planar and octahedral complexes.

UNIT–I Non aqueous solvents

Classification of solvents -properties of ionising solvents -a general study of the typical reactions in liquid ammonia, sulphur dioxide, dinitrogen tetroxide, anhydrous hydrogen fluoride, sulphuric acid and acetic acid. Chemistry of Molten salts as Non-Aqueous Solvents: Solvent properties, solution of metals, complex formation, Unreactivity of molten salts, Low temperature molten salts.

UNIT-II Inorganic hydrides

Transition metal compounds with bonds to hydrogen, carbonyl hydrides and hydride anions. Classification, nomenclature, Wade s Rules, preparation, structure and bonding in boron hydrides (boranes), carboranes, metalloboranes and metallocarboranes.

UNIT–III Coordination Chemistry

Crystal field theory and its limitations, d-orbital splittings, LFSE, spectrochemical series, evidences for metal ligand orbital overlap. Molecular orbital theory and energy level diagrams ($\sigma \& \pi$ bonding), Jahn-Teller distortion. Terms states for dⁿ - ions, energy level diagrams, d-d transitions, Orgel and Tanabe-Sugano diagrams, spin orbit coupling, nephelauxetic effect, charge transfer spectra.

UNIT–IV Reactions of Coordination Complexes - I

Electron transfer reactions; outer and inner sphere processes; atom transfer reaction, complementary and non complementary reaction. Formation and rearrangement of precursor complexes, the bridging ligand, successor complexes, Stereoisomerism in inorganic complexes, isomerism arising out of ligand and ligand conformation Marcus theory.

UNIT – V Reactions of Coordination Complexes - I

Substitution Reactions: Substitution in square planar complexes, reactivity of platinum complexes- Influences of entering, leaving groups- Trans effect, substitution of octahedral complexes of cobalt-S_N1CB.

TOTAL: 60h

Course Outcomes:

- To understand what are polyacids
- To study the stability of the coordination complex
- To familiarize stereochemical aspect of coordination complex
- To know various theories of coordination complex
- To learn the reaction mechanism of coordination complex

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TEXT BOOKS :

- 1. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Co., 1977.
- 2. J. Huheey, Inorganic Chemistry, Harper and Collins, New York, Fourth Edition, 1983.

- 1. R.B.Jordan, Reaction Mechanism of inorganic and Organometallic Systems, Oxford University Press, Third Edition, 1991.
- 2. F.A. Cotton, F.A. Hart, the Heavy Transition Elements, McMillan Co., 1975.

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Course Objective:

- > To understand the fundamental aspects of classical thermodynamics and chemical potential.
- To learn the important aspects of statistical thermodynamics and chemical potential. To study the simultaneous reaction, fast reaction, reaction in solution and the effect of temperature on reaction rate.

UNIT – I Classical thermodynamics

Definition - Fugacity: Determination of Fugacity- By Graphical method, General method, From equation of state, Approximate calculation method-Variation of Fugacity with temperature and pressure. Fugacity of solids and liquids. Mixture of real gases-Fugacity of a gas in a mixture. The concepts of activity and activity coefficients and their determinations. Influence of temperature and pressure on variation of activity and activity coefficients.

Chemical potential - Partial molar properties -Partial molar free energy –Partial molar volume and partial molar heat content –their significance and determination of these quantities. Equilibrium in heterogeneous system. Variation of chemical potential with temperature and pressure. Alternative definition of chemical potential.

UNIT – II Statistical thermodynamics

Concept of thermodynamic probability – distribution of distinguishable and non distinguishable particles. Maxwell – Boltzmann, Fermi – Dirac and Bose- Einstein statistics-Comparison and applications – modes of contribution to energy- Partition function – evaluation of translational, vibrational and rotational, nuclear and electronic partition functions for mono, di atomic and poly atomic ideal gases-thermodynamic functions in terms of partition functions to heat capacities of ideal gases – Law of equipartition energy-heat capacity of solids (Einstein and Debye models).

UNIT – III Chemical Kinetics-I

Simultaneous reaction- A detail study of reversible reaction-First order opposed first order, first order opposed second order reactions-. Effect of temperature on reaction rate Theories of reaction rates- Collision theory of bimolecular gaseous reaction, ACT of bimolecular reactions, Lindemann theory of unimolecular reactions. Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions,

UNIT – IV Chemical Kinetics-II

Kinetics of Chain reactions- general treatment of chain reactions – chain length - Rice Herzfeld mechanism – explosion limits. Kinetics of reaction in solutions- Reactions in solutions – Effect of pressure, dielectric constant and ionic strength on reactions in solutions- Kinetic isotope effects – Linear free energy relationships – Hammett and Taft equations. Study of fast reaction – relaxation methods – temperature and pressure jump method – stopped flow and flash photolysis methods.

UNIT – V Chemical Kinetics-III

Catalysis- Characterstic of catalytic Reaction- Types of Catalysis-Homogenous catalysis-Acid base catalysis – Mechanism of acid base catalysed reactions. Enzyme Catalysis-Mechanism of Enzyme Catalysis. Heterogeneous catalysis- Kinetics of surface reaction – Uni-molecular and Bi-molecular surface reaction, pH dependence of rate constants of catalysed reaction. Langmuir and BET adsorption isotherms.

TOTAL: 60h

Course Outcomes:

- To learn about the Principle and applications of ultraviolet and Woodward Fisher Rule
- To understand the Maxwell's relationships, spontaneity, equibria-Temperature, pressure dependence of thermodynamic quantities
- To know about the concepts of activity and activity coefficients and determination of activity coefficient
- To familiarize the Partial molar properties and its determination
- To learn about the chemical potential and its determination

TEXT BOOKS:

- 1. K.J. Laidler, Chemical Kinetics, Harper and Row, New York, third edition, 1987.
- 2. Rajaram J. and Kuriacose J.C. Kinetics and Mechanism of Chemical Transformation, Mc Millan India Ltd., New Delhi, first edition, 1993.

- 1. S. Glasstone and D.Lewis, Elements of Physical Chemistry, Macmillan, 2nd Edition, 1995.
- 2. P.W. Atkins, Physical Chemistry, Oxford University Press, 5th edition, 1995.

18PMSG11PHYSICAL CHEMISTRY - PRACTICAL I0 0 6 3Course Objective:

- > To understand and analyse the kinetic and thermodynamic. aspects of reactions.
- > To learn the significance of potentiometric and conductometric titrations.

Non Electrical experiments:

- 1. Determination of relative strength of the given 2 acids catalysed by methyl acetate.
- 2. Determine the temperature coefficient & energy of activation of hydrolysis of methyl acetate.
- 3. Construction of Phase diagram for a simple binary system.
- 4. Determination of rate constant & order of reaction between K₂S₂O₈ & KI
- 5. Study the primary salt effect on the Kinetics of ionic reactions & test the Bronsted relationship ($K_2S_2O_8 + KI$)
- 6. Determination of equilibrium constant of the reaction between I_2 + KI by Partition method.
- 7. Study the adsorption of acetic acid by charcoal (Fruendlich isotherm).

Electrical Experiments:

I. Potentiometric titrations:

- 1. Strong acid Vs Strong Base
- 2. Weak acid Vs Strong Base
- 3. Mixture of acid Vs Strong Base
- 4. Halides Vs AgNO₃
- 5. Mixture of halides Vs AgNO₃
- 6. Redox Titration
- a. FeSO₄ Vs K₂Cr₂O₇ b. KI Vs KMnO₄
- 7. Determination of pKa of a weak acid using Henderson equation.

II. Conductometric titrations:

- 1. Strong acid Vs Strong base.
- 2. Strong acid & weak acid Vs Strong base (Mixture of acids Vs Strong base)
- 3. Weak acid Vs Strong base.
- 4. Determination of cell constant and verification of Debye-Huckel Onsager equation for strong electrolyte.
- 5. Determination of dissociation constant of weak electrolyte by conductivity method.

TOTAL: 90h

Course Outcomes:

- The student will be learning the concept of electrical experiments
- To learn to construct phase diagram
- To understand the concept distribution coefficient
- To know how to hydrolyze ester
- To study the reaction kinetics

TEXT BOOKS:

- 1. P. S. Raghavan, B. Viswanathan, Practical Physical Chemistry, Viva books Private Limited, New Delhi, 2005.
- 2. B.D. Khosla and V.S. Garg, Senior Practical Physical Chemistry, R. Chand and Co., New Delhi, 1998.

- 1. A. Findary, T.A. Kitchner Practical physical chemistry, Longmans, Green and Co., 1997.
- 2. J.M. Wilson, K.J. Newcombe, A.R. Denko. R.M.W. richett, Experiments in Physical Chemistry, Pergamon Press, 2007.

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Course Objective:

- > To study mechanisms of addition reactions, elimination reactions, oxidation and reduction reactions and reactions involving rearrangements.
- > To understand the conformation of some important organic compounds.

UNIT – I Addition to carbon - carbon and carbon-hetero multiple bonds

Electrophilic, nucleophilic and neighbouring group participation mechanism-Addition of halogen and nitrosyl chloride to olefins. Hydration of olefins and acetylenes. Hydroboration, Hydroxylations, Michael addition, Diels Alder reaction, 1,3-dipolar additions.

Carbenes and their addition to double bonds-Simmon Smith reaction, Mannich, Stobbe, Darzen, Wittig, Wittig – Horner, Tebbe and Benzoin reactions. Stereochemical aspects to be studied wherever applicable. Nitrene : methods for generating nitrenes and their reactions.

UNIT – II Elimination Reactions

 E_1 , E_2 and E_1cB mechanism- E_1 , E_2 and E_1cB Spectrum—orientation of the double bond – Hoffmann and Saytzeff rule s- competition between elimination and substitution. Typical elimination reactions – dehydration, dehydrohalogenation and dehalogenation. Stereochemistry of E_2 eliminations in cyclohexane systems. Mechanism of pyrolytic elimination. Chugaev and Cope eliminations.

UNIT – III Molecular Rearrangements

A detailed study with suitable examples of the mechanism of the following rearrangements: Pinacol-pinacolone(examples other than tetra methyl ethylene glycol)-Wagner-Meerwein, Demjanov, dienone – phenone, Favorskii, Lossen, Baeyer – Villiger, Dakin Rearrangement, Wolf, Stevens (in cyclic systems) and Von Richter rearrangements.

UNIT – IV Oxidation and Reduction

Mechanisms – study of the following oxidation reactions–oxidation of alcohols using chromium (Jones oxidation, Collins & Sarrett reagents, PCC & PDC) -use of DMS (Corey-Kim Oxidation), DMSO in oxidizing alcohols (Pfitzner-Moffatt Oxidation, Kornblum Oxidation, Swern Oxidation), Dess-Martin Oxidation- oxidation of alkene to carbonyl (OsO_4 , $Pb(OAc)_4$, Ozonolysis), SeO₂. Reductions : selectivity in reduction of 4-T- Butyl cyclo hexanone using selectrides hydride reductions – synthetic importance of Clemmenson and Wolff- Kishner reductions- modifications of Wolff-Kishner reduction – Birch reduction , MPV reduction.

UNIT – V Conformational Analysis

Conformation of some simple 1,2 disubstituted ethane derivatives. Conformational analysis of disubstituted cyclohexanes and their stereochemical features (geometric and optical isomerism (if shown) by these derivatives). Conformation and reactivity of substituted cyclohexanols (oxidation and acylation), cyclohexanones (reduction) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis) Conformation and stereochemistry of *cis* and *trans* decalin and 9-methyldecalin.

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Course Outcomes:

- The learn the principle of addition reaction
- To study the mechanism of familiar organic name reactions followed by addition mechanism
- To learn the concepts of elimination reaction
- To understand the detail mechanism of various types of molecular rearrangement
- To study the various familiar oxidation reactions like oppenaur oxidation

TEXT BOOKS:

- R.O.C. Norman, Principles of Organic Synthesis, Chapman and Hall, London, 2nd 1980.
- 2. Francis A. Carey, Richard J. Sundberg, Advanced Organic Chemistry-Part B Reactions and Synthesis, Plenum Press, 3rd Edition, 1990.

- **1.** S.M. Mukherji and S.P. Singh, Organic Reaction Mechanism, Macmillan India Ltd., 1990.
- 2. P.S. Kalsi, Textbook of Organic Chemistry, Macmillan India Ltd., 1999.

INORGANIC CHEMISTRY-II

Course Objective:

- > To learn about some organometallic compounds and their applications in industry.
- > To learn the applications of IR, Raman, NMR ESR and Massbauer techniques.
- > To study the salient features of solid state chemistry.

UNIT –I Metallocenes

Alkyls and arene complexes; metalation, bonding in metal carbonyls and nitrosyls, chain and cyclic donors, olefin, acetylene and allyl systems, synthesis, structure and bonding metallocenes.

UNIT –II Organometallic reactions-I

Organometallic reactions - Association, Carbonylation, decarbonylation, Insertion, Elimination and rearrangement. Examples, mechanisms and application.

UNIT –III Organo metallic Reactions

Catalysis-Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalysts (oxoprocess), oxidation of olefins to aldehydes and ketones (Wacker process) polymersiation (Zeigler-Natta catalyst); cyclo oligomerisation of acetylene using nickel catalyst (Reppes' catalyst)-Synthetic Gasoline-mobil Reaction.

UNIT-IV Solid state - I

Structure of solids: Comparison of X-ray, Neutron and Electron diffraction, structure of ZnS, Rutile, Pervoskite, Cadmium iodide and Nickel arsenide: Spinels and inverse spinels: defects in solids, non-stochiometric compounds.

UNIT-V Solid state - II

Band theory, semiconductors, superconductors, solid state electrolytes, types of magnetic behaviour, Dia, Para, Ferro, Antiferro and ferri magnetism: Hysterisis, Solid state lasers, inorganic Phosphors.

Course Outcomes:

- To learn what are metallocenes
- To understand various types of metallocenes synthesis, structure and bonding
- To learn what are organometallics
- To know the uses of various catalyst Wilkinson, Reppes, Zeiglar Natta
- To understand Oxo and wacker process

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TOTAL: 60h

TEXT BOOKS:

- 1. J.E. Huheey, Inorganic Chemistry Principles, Structure and Reactivity: Harper Collins, New York, 4th Edition,1993.
- 2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry- A Comprehensive Text, John Wiley and Sons, 5th Edition,1998.
- 3. K. F. Purcell and J.C. Kotz, Inorganic Chemistry, WB Saunders Co., USA 1977.

- 1. M.C. Day and J. Selbin, Theoretical Inorganic Chemistry, Van Nostrand Co., New York, 1974
- 2. D.F. Shrivers, P.W. Atkins and C.H. Langfor, Inorganic Chemistry, CH Langford, 1990.
- 3. N.N. Greenwood and Earnshaw, Chemistry of the Elements, Pergamon Press New York,1984.

PHYSICAL CHEMISTRY-II

- > To study fundamental aspects of classical mechanics, the harmonic oscillator, rigid rotor and Born – Oppenheimer approximation.
- To learn about the general aspects of group theory.

UNIT – I **Quantum Chemistry-I**

Classical mechanics- reason for failure- Basic principles of quantum mechanics. Atomic spectra, block body radiation, photoelectric effect-, Bohr's correspondence principledeBroglie wave particle duality- Heisenberg uncertainty principle.

Eigen Values and Eigen Functions. Quantum mechanical postulates – the Schrodinger equation – elementary applications of Schrodinger's equation – the particle in a box (one and three dimensional cases)

UNIT – II **Quantum Chemistry- II**

The harmonic oscillator – the rigid rotor- the hydrogen atom – Schrodinger equation for hydrogen atom –unnormalised and normalised wave equations-the solution- the origin of quantum numbers (Angular momentum and spin)- their physical significance. Helium atom and Pauli's exclusion principle.

UNIT – III **Quantum Chemistry- III**

Approximation methods – Variation and Perturbation theorem, methods – application to hydrogen, helium atoms - R, S Coupling and term symbols for atoms. Born-Oppenheimer approximation –valence bond theory for hydrogen molecule –LCAO-MO theory for di and poly atomic molecules- concept of hybridization –Huckel theory for conjugated molecules (ethylene, butadiene and benzene) - semi-empirical methods-Slater orbital and HF-SCF methods.

UNIT-IV Group theory-I

Symmetry elements and symmetry operations – Mathematical rules for the formation of a group- Definition and classification of Point groups – Identification and determination – Matrix representations- Reducible and irreducible representations- Similarity transformation -Orthogonality theorem and its consequences - Character table- Construction of Character table for C_{2V} and C_{3V} point group. Determination of symmetry of hybrid orbitals-Symmetry of hybrid orbitals in non linear molecules (H₂O,CH₄,XeF₄,BF₃,SF₆ and NH₃).

UNIT – V Group theory-II

Molecular vibrations -Direct product representation-Determination – IR and Raman activity of vibrational modes in non linear molecules (H₂O, CH₄,XeF₄,BF₃,SF₆ and NH₃). Mutual exclusion principle. Symmetry selection rules of infrared and Raman Spectra. Selection rules for electronic transitions. Symmetry of molecular orbitals and electronic states of HCHO. Selection rules for electronic transitions of HCHO.

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TOTAL: 60h

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Course Objective:

Course Outcomes:

- To learn the posulates of Quantum mechanics
- To know the basisc principles of quntum mechanics
- To understand Hessinberg uncertainity principle
- To Familaries approximation methods in quntum chemistry
- To understand importants of schordingers wave equations

TEXT BOOKS:

- 1. R. Anantharaman, Fundamentals of Quantum chemistry, Macmillan India Limited 2001.
- 2. I.N. Levine, Quantum Chemistry, Prentice Hall India, 4th edition, 1994.
- 3. Ramakrishnan, M.S Gopinathan, Group Theory in Chemistry, Vishal Publications, New Delhi,1988.
- 4. K. V.Raman, Group theory and its applications to Chemistry, Tata McGrawHill, New Delhi, 1990.

- 1. D.A. McQuarrie, Quantum chemistry, University Science Books, Mil Valley, California,1983.
- 2. T.N. Levine, Quantum Chemistry, Allyn and Bacon, Boston, 1983.

15PMSG21ORGANIC CHEMISTRY – PRACTICAL II0 0 6 3

Course Objective:

- > To know the techniques of separating organic compounds from the mixture.
- > To learn the methods of crystallization and the method of purification.
- I. Identification of components in a two component mixture and preparation of their derivatives.
- 1. Acid substance and neutral substance
- 2. Basic substance and neutral substance
- 3. Phenolic substance and neutral substance
- 4. Acid substance and phenolic substance
- 5. Phenolic substance and basic substance
- **II.** Determination of b.pt. /m.pt. for components and m.pt. for the derivatives.

III. Preparations:

- 1. p-Nitrobenzoic acid from p-Nitrotoluene
- 2. Anthroquinone from anthracene
- 3. Benzhydrol from benzophenone
- 4. m-ntroaniline from m-dinitrobenzene
- 5. 1,2,3,4-Tetrahydrocarbazole from cyclohexanone
- 6. Methyl orange from sulphanilic acid.
- 7. Iodobenzene from aniline

TOTAL: 90h

Course Outcomes:

- To familiarize the solubility nature of organic substances of different functional group.
- To learn the pilot separation of bimixtures .
- To familiarize the systematic producers organic substances analysis
- To learn two stage preparation involving molecular rearrangement oxidation .
- To know the preparation involving nitration and bromination

TEXT BOOKS:

1. N.S. Gnanapragasam, G. Ramamurthy, Organic Chemistry Lab Manual, S.Vishwanath Printers & Publishers Pvt. Ltd., Chennai, 2010. Day & Underwood, Quantitative Analysis, Prentice Hall of India Pvt. Ltd., New Delhi. 6th Edition,2004.

- Arthur I.Vogel, Elementary Practical Organic Chemistry (Part 1, 2 and 3), CBS Publishers and Distributors, New Delhi,5th Edition, 1989.
- J Leonard, B Lygo, G Procter, "Advanced Practical Organic Chemistry", Stanley Thornes (Publishers) Ltd., First Indian Edition, 2004.

15PMSG22 ANALYTICAL CHEMISTRY – PRACTICAL III 0063

Course Objective:

- > To learn the separation technique and the instrumentation in the analysis of metals.
- > To understand the volumetric estimations of organic compounds.

Inorganic Experiments

I. Quantitative analysis

Gravimetric analysis of mixtures of

- 1. Iron and magnesium
- 2. Iron and nickel + Cr
- 3. Copper and nickel and
- 4. Copper and Zinc.
- 5. Copper and Tin.

II. Analysis of Ores

- 1. Dolomite
- 2. Copper Pyrites
- 3. Pyrollusite

III. List of spectra to be given for interpretation.

- 1. ³¹P NMR Spectra of methylphosphate
- 2. ³¹P NMR Spectra of HPF₂
- 3. ¹⁹F NMR Spectra of CIF₃
- 4. Expanded high resolution 1H NMR spectra of

(N-propylisonitrosoacetylacetoneiminato) (acetylacetoneiminato)Nicketl(II)

- 5. ESR Spectra of the aqueous $ON(SO_3)_2^{2^2}$ ion
- 6. ESR Spectra of the $[Mn(H_2O)_6]^{2+}$ ion
- 7. IR Spectra of the nitro and nitritopentaminecobalt (III) chloride
- 8. IR Spectra of carbonyls
- 9. Mossbauer spectra of FeSO₄.7H₂O
- 10. Mossbauer spectra of $[Fe(CN)_6]^{3-1}$

Organic Experiments:

I) Any Six Preparations from the following involving two stages:

1. Sym-Tribromo benzene from aniline.

- 2. Benzanilide from benzophenone.
- 3. *m*-Nitrobenzoic acid from methylbenzoate
- 4. 2,4-Dinitrobenzoic acid from p-nitrotoluene
- 5. m-nitrobenzoic acid from benzaldehyde
- 6. Benzil from benzaldehyde
- 7. Anthaquinone from phthalic anhydride
- 8. Phthalide from phthalic anhydride
- 9. 2-phenyl indole from phenylhydrazine
- 10. 2,4-Dinitrophenyl hydrazine from p-nitrochlorobenzene.

II) Any Five Estimations:

- 1. Estimation of aniline.
- 2. Estimation of Phenol
- 3. Estimation of glucose
- 4. Estimation of amino group
- 5. Estimation of amide group
- 6. Saponification of fat or an oil
- 7. Iodine value of an oil
- 8. Estimation of sulphur in an organic compound
- 9. Estimation of methyl ketone.

III) Special Interpretation of organic compounds, UV,IR, PMR and Mass spectra of 10 compounds

1.	1,3,5-Trimethylbenzene	2. Isopropyl alcohol
3.	Pinacolone	4. Acetone
5.	2-N, N-Dimethylamino thanol	6. Benzyl bromide
7.	Pyridine	8. Phenylacetone
9.	Cinnamaldehyde	10. 1,3-dibromo-1, 1-dichloropropene

TOTAL:90h

Course Outcomes:

• To learn the technique of separating the one cationic mixture by precipitation and estimating another by gravimetric.

- To learn the technique of precipitation of cations as glyoximates, oxinates and sulphates and estimating them by gravimetrically.
- To involve the techniques of time management of multi stage organic preparation.
- To learn the multi stage preparation by electrophilic substitution, oxidation and hydrolysis.
- To witness the utility of protecting and deprotecting steric hindering groups.

TEXT BOOKS:

- 1. Gary D. Christian, "Analytical Chemistry", John Wiely & Sons, INC, New York, Fifth Edition, 1994.
- V.K. Ahluwalia, Sunita Dhingra, "Comprehensive Practical Organic Chemistry Qualitative Analysis", University Press Private Limited, India, First Indian Edition, 2010.

- 1. John H. Kennedy, "Analytical Chemistry: Practice", Saunders College Publishing, New York, Second Edition, 1990.
- 2. Russell.S.Drago, Physical Methods in Inorganic Chemistry, West Press Private Limited, New Delhi, 1965.

Course Objective:

- To gain practical experience by working in a professional chemistry -related environment.
- To demonstrate an ability to work independently and utilize principles of chemistry to solve real-world problems.

Course Requirements:

- Students wishing to receive credit for internship are required to find, apply for, and be selected for a chemistry or materials related internship position with an organization of their choice. They will then need to seek permission by the Department Chair to register for the appropriate internship course.
- The student must complete at least 90 hr of work during the semester for each hour of academic credit awarded, and these work hours must be completed during the term (odd or even semester vacation) in which the student is registered for the internship course.
- After the student has completed the internship, the student must submit the final evaluation report of the internship experience and 20 minute presentation to department at conclusion of semester. The Department Chair and class instructor will allot the marks for the internship evaluation report.

Course Outcomes:

- To know the various types of industries.
- To learn the procedure of identifying, approaching, applying and getting approval of internship from a leading industry.
- To witness the entire work area of the industry.
- To understand the nature of job involved in the various sector of the industry.
- To adapt with the working people.

ORGANIC CHEMISTRY-III

Course Objective:

- To study the structure elucidation of organic molecules using NMR, Mass spectroscopy and IR spectroscopy.
- > To know about the general aspects of organic photochemistry.
- > To learn about Heterocycles, terpenoids, steroids and cholesterol.

UNIT-I Introduction to photochemistry

Basic concepts of organic photochemistry: Thermal versus photochemical reactions – electronic excitations – n – π^* and π – π^* transitions, singlet and triplet energy states – comparison of energies, lifetimes and reactivates; allowed and forbidden transitions; fluorescence, phosphorescence and internal conversion – intersystem crossing; Jablonski diagram; quantum yields and their determination; sensitization and quenching

UNIT-II Organic Photochemistry

Photochemical reactions of saturated ketones – Norrish Type I and Norrish Type II reaction; photoreduction of ketone, photoaddition reactions, Paterno Buchi reaction. Photochemistry of simple olefins – cis – trans isomerization, 1,3-dienes, 1,4- dienes, di – pi methane rearrangement, 1,5 – dienes – sigmatropic rearrangement. Photooxidation – Formation of peroxy compounds – oxidative couplings – Barton reaction. Photo rearrangements : Photo – Fries rearrangement and Photo rearrangement of 2,5 – Cyclohexadienones.

UNIT-III Pericyclic Reactions

Pericyclic reactions- classification –orbital symmetry-Woodward Hoffman rules-Analysis of electrocyclic, inter conversion of hexatrienes to cyclohexadienes. Cyclo addition and sigmatropic reactions-correlations diagram for butadiene-cyclobutene system. Structure of butylene, a fluxional molecule –Cope and Claissen rearrangements.

UNIT-IV Heterocycles, and Terpenoids

Imidazole, oxazole, thiazole, flavones, isoflavones, anthocyanins, pyrimidines (cytocine and uracil only) and purines (adenine, guanine only). Synthesis of parent and simple (alkyl or aryl substituted derivates are expected). Synthesis of vitamin A1 (Reformatsky and Wittig reaction methods only).

UNIT-V Steroids

Classification with examples, nomenclature of steroids; Structure, Conversion of cholesterol to progesterone, estrone and testosterone. Elucidation of structure of cholesterol (by chemical degradation).

TOTAL: 60h

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Course Outcomes:

- To learn principle and application of UV-Visible and IR Spectroscopy.
- To practice the calculation of λ max using woodward fischer rule.
- To learn the principle behind NMR Spectroscopy H¹, C¹³, P³¹.
- To understand the principle behind Mass spectroscopy and its applications.
- To know what is ORD and CD.

TEXT BOOKS:

- 1. I.L. Finar, Organic Chemistry, ELBS Publication, 5th Edition, 2000.
- B.K. Sharma, Instrumental methods of Chemical analysis, Goel Publishing House, 24th Edition, 2005.

- 1. J. Dyer, Application of absorption spectroscopy of organic compounds, Prentice-Hall India Pvt. New Delhi, 2008
- 2. R. M. Silverstein, G. C. Bassler and Monsil, Spectrometric identification of Organic compounds, John Wiley and Sons, New York, 1998.

INORGANIC CHEMISTRY-III

Course Objective:

18CMSG32

> To study the biological aspects, metalloenzymes, oxygen carriers, nitrogen fixation, photosynthesis and toxicity of heavy metals.

UNIT – I Basic concepts of Bioinorganic Chemistry

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

UNIT – II Enzymes

Essential and trace metal ions.Coenzymes – Vitamin B coenzymes, carboxy peptidase and Superoxide dismutase. Heme – enzyme – Peroxidase and catalases.

UNIT – III Hemeproteins

Oxygen carriers – Hemeproteins – Hemoglobin, myoglobin – Structure Oxygenation and Stereochemistry – Bohr effect. Non-heme oxygen carriers – Hemerythrin and hemocyanin-Iron storage and transport proteins.

UNIT – IV Nitrogen fixation and biological redox systems 12

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

Iron – sulphur proteins – rubredoxin and ferredoxin.Photosynthesis and chlorophyll's.

UNIT – V Bio analytical Chemistry

Bio analytical Chemistry, Toxicity & medicine, Toxicity of Hg, Cd, Zn, Pb, As, Sb. Anti cancer agents, Metal ion poisoning: Failure of metal ion control systems, role of metal ion Diagnosis and treatment – use of radio isotopes; Pollution studies: Effluents and treatment. Inorganic plant nutrition and indicator plants for mineral exploration.

Course Outcomes:

- To learn the basic concepts of bio inorganic chemistry.
- To learn what are the essential metal ions and their role in biological system.
- To learn Heme proteins and porphyrin complexes.
- To understand biological redox systems, metal clusters and nitrogen fixation
- To know the concepts of bio analytical chemistry.

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TOTAL: 60h

TEXT BOOKS:

- 1. Williams, D.R., Introduction to Bioinorganic Chemistry, C.C.Thomas, Springfield, 1976.
- 2. M.Satake and Y.Mido, Bioinorganic Chemistry, Discovery Publishing House, New Delhi, 1996.

- 1. G.Eichron, G., Inorganic Bio-Chemistry, Vol. I and II, Elsevier, 1973.
- 2. J.Huheey, Inorganic Chemistry, Harper and Collins, New York, fourth Edition, 1993.

> To analyse the structure of different compounds by using different Techniques.

Mean ionic activity and mean ionic activity coefficient – concepts ionic strength. Nernst equation- redox system- electrochemical cell- Electrolytic conductance- Kohlraush's law and its applications, ionic equilibria. Debye- Huckel theory of strong electrolytes – Determination of activity coefficient by electrical method –Debye-Huckel limiting law qualitative and quantitative verification – Limitation of Debye –Huckel theory at appreciable concentration –

PHYSICAL CHEMISTRY-III

To learn the electrochemical aspects of reactions

Electro Chemistry-I

Electro Chemistry-II

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Electrode –electrolyte interface – adsorption at electrified interface- electrical double layer – Electrocapillary phenomenon – Lippmann Equation – Structure of double layers – Helmholtz – Perrin- Guoy-Chapman and Stern model of electrical double layers.

UNIT-III Electro Chemistry-III

Mechanism of electrode reaction – Polarisation and overpotential – the Butler Volmer equation for one step and multi step electron transfer reaction – Significance of exchange current density and symmetric factor-transfer coefficient and its significance – Mechanism of the hydrogen and oxygen evolution reactions.

UNIT-IV Spectroscopy-I

Interaction of matter with radiation – Einstein's theory of transition probability – rotation spectroscopy of a rigid rotor – non- rigid rotor – di atomic and poly atomic molecules. Vibrational spectroscopy – harmonic Oscillator – anharmonicity – Vibrational spectra of poly atomic molecules- Vibrational frequencies - group frequencies – Vibrational coupling overtones – Fermi resonance. Raman Spectra.

UNIT-V Spectroscopy-II

Equation of motion of spin in magnetic fields –Chemical shift – spin-spin coupling –NMR of simple AX and AMX type molecules –calculation of coupling constants- ¹³C, ¹⁹F, ³¹P NMR spectra – applications – a brief discussion of Fourier transform resonance Spectroscopy.

TOTAL: 60h

Course Outcomes:

- To learn the concepts of the activity coefficients and electrochemical cell.
- To study the theory of Debye Huckel rule, limitations and its applications.
- To know the structure of electrical double layers of Helmholtz, perrin-guoy-chapman.
- To know the adsorption of electrolyte interface.
- To practice the mechanism of hydrogen and oxygen evolution reaction.

18CMG33

UNIT-I

UNIT-II

Course Objective:

- 1. S. Glasstone, Principles and Applications to Electrochemistry, Chapman and Hall, 1991.
- 2. D. R. Crow, Introduction to Electrochemistry, Affiliated East West Press, New Delhi, 1960.

- 1. P. H. Rieger, Electrochemistry, chapman and hall, New York, 1994.
- 2. G. Aruldas, Molecular Structure and Spectroscopy, Prentice Hall, 2002
- 3. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1962.

18PMSG31 INORGANIC CHEMISTRY – PRACTICAL IV 0063

Course Objective:

- > To learn the quantitative determination of compound by volumetric titration method.
- > To learn the qualitative analysis of a given salt mixture.

I. Volumetric Estimations :

- 1. Estimation of Zinc
- 2. Estimation of Magnesium
- 3. Estimation of Calcium
- 4. Estimation of Nickel

II. Colorimetric analysis:

- 5. Estimation of iron
- 6. Estimation of nickel
- 7. Estimation of manganese
- 8. Estimation of copper.

III. Qualitative analysis:

- 9. Analysis of Salt mixture-I (W, Se, Pb, Cu)
- 10. Analysis of Salt mixture- II (Te, Th, Al, Fe)
- 11. Analysis of Salt mixture- III (Ti, Zr, Mn,Co)
- 12. Analysis of Salt mixture- IV (Ce, V, Ni, Zn)

TOTAL: 90h

Course Outcomes:

- To know about the Volumetric analysis of cations.
- To identify the simple cations
- The communication of the results of scientific experiments in oral reports and written reports
- The chemical literature and to read and understand technical literature related to the discipline
- To analysis the simple Inorganic salt mixture

TEXT BOOKS:

- 1) Jeyavathana Samuel, Chemistry Practical Book, G.G.Printers, Chennai, 2012.
- 2) Vickie.M.Williamson, M.Larry Peck, Lab manual for General Chemistry, Cengage Learning India Private Limited, New Delhi, 2009.

- 1) V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Publishing Company, Chennai, third edition, 1974.
- 2) Vogel's "Textbook of Quantitative chemical Analysis", Pearson Education Ltd. Sixth Edition, 2008

18CMSG41 ELECTROANALYTICAL AND SEPARATION TECHNIQUES

Course Objective:

- > To understand the electrolytic conductance, electrode and mechanism of electrode reaction.
- To study the interaction of matter with radiation.
- \succ To know about B_c, K_F, pNMR Spectroscopy and fourier transform resonance spectroscopy

UNIT – I Analytical Techniques –I 15

Polarography – theory, apparatus, DME, Diffusion, Kinetic and catalytic currents, Current - voltage curves for reversible and irreversible system, qualitative and quantitative applications to inorganic systems.

UNIT – II Analytical Techniques –II

Amperometric titrations - theory, apparatus, types of titration curves, successive titrations and indicator electrodes – Applications. Cyclic voltammetry - theory, application to inorganic systems-Coulometry.

UNIT – III Introduction to Chromatography

Adsorption and partition chromatography, definition of terms, techniques and chemical concept of column, paper, TLC and HPTLC

UNIT – IV Separation Technique-I

Chromatography: Gas-liquid Chromatography, Principles, Retention Volumes, Instrumentation, Carrier Gas, Columns, Stationary Phase, Detectors, Thermal Conductivity, Flame Ionization, Electron Capture, Application of G.L.C.

UNIT – V Separation Technique-II

High Performance Liquid chromatography: Scope, Column efficiency, Instrumentation, Pumping Systems, Columns, Column packing, Detectors, Applications. Ion exchange and gel – permeation chromatography.

Course Outcomes:

- To learn about the definition of Adsorption and partition chromatography
- To understand the Column, Paper, Thin Layer Chromatography
- To know about the High Performance Thin Layer Chromatography
- To familiarize the Two dimensional Paper Chromatography, Reverse phase paper chromatography.
- To learn about the Gas-liquid Chromatography. ٠

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TOTAL: 75 h

- 1. J. Huheey, Inorganic Chemistry, Harper and Collins, New York, IV Edition, 1983.
- 2. H.J. Arnikar, Nuclear Chemistry, Wiley Eastern Co., II Edition, 1987.

- 1. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry- A Comprehensive Text, John Wiley and Sons, V Edition, 1998.
- 2. K. F. Purcell and J.C. Kotz, Inorganic Chemistry, WB Saunders Co., USA, 1977

To learn about the basic concept of project work. To know about designing new experiments and carry out the experiments. To know about the various characterization techniques used to characterize the synthesized compounds. To know about the necessities of literature survey and to learn about writing dissertation of project work.

NOTE

- 1. Review of Chemical literature and documentation.
- 2. During the fourth semester the project work may be carried out either in industries/ National laboratories/R & D centers/in the university lab.

TOTAL: 24 h

Course Outcomes:

- To identify the topic with the consideration feasibility.
- To learn the procedure of literature survey of the concered topic.
- To derive a plan for executing the work in the stipulated time with maximum efficiency and success.
- The intensive exposure to industry as a first time experience.
- Understanding different sectors of an industry and the functionaries of each sector.

Syllabus Discipline Specific Elective Courses

To study the types of polymerization, polymerization techniques, crystallinity in polymers, applications of polymer, polymer degradation and additives for polymers.

UNIT –I Basic Concepts of Polymers.

Monomer, Repeating unit, degree of polymerization. Classification of polymers, Stereochemistry of polymer, nomenclature of stereo regular polymers. Types of polymerization - Chain polymerization, free radical polymerization; ionic polymerization; Coordination polymerization and Ziegler Natta catalyst.

UNIT- II Types of Polymerisation

Step polymerization, ring opening polymerization. Co polymerization, random, block and graft co polymers- preparation. Plastics – Types of plastics - Rubber – Natural and synthetic rubber - Vulcanisation of rubber.

Polymerisation techniques; bulk, solution, suspension and emulsion polymerization.

UNIT- III Molecular Weight and Glass Transition Temperature

Measurement of molecular weight and size; number average and weight average molecular weights. Glass transition temperature, concepts of glass transition temperature and associated properties.

UNIT- IV Glassy Solids and Polymer Crystallization

Glassy solids and glass transition, factors influencing glass transition temperature (Tg). Crystallinity in polymers; Polymer crystallization, structural and other factors affecting crystallisability, effect of crystallinity on the properties of polymers.

UNIT –V Types of Polymers and Polymer Degradation

Synthetic resins and plastics; Manufacture and applications of polyethylene, PVC, Teflon, poly styrene, polymethylmethacrylate, poly urethane, phenol – formaldehyde resins, urea- formaldehyde resins and epoxy polymers.

Polymer degradation: Types of degradation- thermal, mechanical, photo, hydrolytic and oxidative degradations. Additives for polymers: Fillers, plasticizers, thermal stabilizers, photo stabilizers, anti oxidants and colourants.

TOTAL: 45h

Course Outcomes:

- To know about basic ideas of polymers like monomer, repeat unit and degree of polymerization.
- To learn about the stereochemistry and nomenclature of polymers.
- To understand the various types of polymerization.
- To know the preparation and polymerization techniques.
- To understand the number average and weight average molecular weights.
- To learn about the concepts of glass transition temperature.
- To know the various factors influencing glass transition temperature.
- To understand the principle of crystallinity.

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Fred. W. Billmeyer, Text Book of Polymer Science, John Wiley & Sons, Third Edition, 2007.
R. V. Gowariker, Polymer Science, New Age International Publication, 2006.

- 1. A. Ravve, Principles of Polymer Chemistry, Springer New York, Third Edition, 2012.
- 2. R. J. Young and P. A. Powell, Introduction to Polymers, CRC Press, Third Edition, 1991.

To understand the basic principles, instrumentation and applications of UV-visible spectroscopy, mass, IR Spectroscopy, Raman spectroscopy, calorimetric analysis and resonance spectroscopy.

UNIT- I Techniques of UV- Visible spectroscopy and Infrared Spectroscopy

Colourimetric analysis and UV- Visible spectroscopy: Beer Lambert's law, Principles of single and double beam instruments – applications for analysis of inorganic and organic samples.

Infrared spectrophotometric analysis - principle and instrumentation and molecular structure determination.

UNIT – II **Raman Spectra and Nuclear Magnetic Resonance**

Raman Spectra – principle, basic instrumentation – structural analysis.

Nuclear Magnetic Resonance - Principle, instrumentation, structure determination, NMR of ¹H, ¹³C, ³¹P, ¹⁹F.

UNIT – III Electron Spin Resonance and Mass Spectrometry

Electron Spin Resonance - Principle, instrumentation, applications to coordination compounds.

Mass Spectrometry – Principle, basic instrumentation, fragmentation patterns – organic molecular structural determination.

UNIT- IV Thermogravimetric Analysis

Thermo gravimetric and differential thermal analysis, DSC thermometric titrations, differential scanning colourimetry - principles, basic instrumentation properties and applications.

UNIT – V Atomic Absorption and Photoelectron Spectroscopy

Atomic absorption spectroscopy: Theory, Atomizers, Flame and Electro thermal. Radiation sources, Instrumentation, spectral and chemical interferences, application.

Photoelectron spectroscopy (UV and X-Ray) –photo electron spectra Koopman's theorem, fine structure in PES, chemical shift and correlation with electronic charges.

Course Outcomes:

- To learn about the Colourimetric analysis
- To understand the UV spectroscopy
- To know about the Mass Spectrometry Principle, basic instrumentation, fragmentation patterns
- To familiarize the Thermogravimetric Analysis
- To learn about the Infrared spectrophotometric analysis principle and instrumentation and molecular structure determination.
- To learn the principle, instrumentation and applications of Raman Spectra
- To know about the principle, instrumentation and applications of NMR Spectra
- To know the detail study of the Electron Spin Resonance and Mass Spectra.

TOTAL: 45h

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• To learn about the Atomic Absorption and Photoelectron Spectroscopy

TEXT BOOKS:

- 1. D. A. Skoog and D. M. West, Fundamentals of Analytical Chemistry, IV Edition, Old Reinhord & Winston, Publication, 1982. (Refer for UNIT V).
- 2. B. K. Sharma, Instrumental methods of Chemical analysis, Goel Publishing House, 4th Edition, 2005. (Refer for UNIT I, II, III)
- 3. Gurdeep R. Chatwal, Sham K. Anand, Instrumental Methods of Chemical Analysis, Himalay Publ, 1979.(Refer for UNIT IV)

- 1. Willard Merrit, Dean and Settle, Instrumental methods of analysis, VI Edition, CBS Publ, 1986.
- A. I. Vogel, Textbook of Qualitative Inorganic Analysis, III Edition, ELBS, 1976 Old Reinhord & Winston, Publication, 1982.

SEPARATION TECHNIQUES

Course Objective:

- > To study Isalient features of thermal methods and atomic absorption spectroscopy..
- > To study the general features of chromotographs and their Basic principles.
- > To understand HPLC Ion exchange and gel permeation chromotograpy.

UNIT- I Chromatographic Techniques

Adsorption and partition chromatography- definition of terms- Techniques and applications - Column, Paper, Thin Layer and High Performance Thin Layer Chromatography, Retention Factor, Two dimensional Paper Chromatography, Reverse phase paper chromatography.

UNIT-II Gas Liquid Chromatography

Chromatography: Gas-liquid Chromatography, Principles, Retention Volumes, Instrumentation, Carrier Gas, Columns, Stationary Phase, types of Detectors, Thermal Conductivity, Flame Ionization, Electron Capture, Retention time, Application of G.L.C.

UNIT-III High Performance Liquid chromatography

High Performance Liquid chromatography: Scope, Column efficiency, Instrumentation, Pumping Systems, Columns, Column packing, Detectors, Applications. Ion exchange and gel – permeation chromatography. Standard deviation and correlation coefficient.

UNIT- IV Ion Exchange Chromatography

Basic principle, instrumentation and application of Ion-Exchange chromatography (IEC).

UNIT V Gel Permeation Chromatography

Basic principle, instrumentation and application of Gel Permeation chromatography (GPC). Standard deviation and correlation coefficient.

Course Outcomes:

- To learn the basic principles of chromatography.
- To know about the various techniques involved in chromatography.
- To understand the applications of gas liquid chromatography.
- To know about scope and instrumentation of high performance liquid chromatography.
- To know about scope and column efficiency of high performance liquid chromatography.
- To learn about standard deviation and correlation coefficient of high liquid chromatography.
- To understand the concepts of gel permeation chromatography
- To learn standard deviation and correlation coefficient of gel permeation chromatography

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TOTAL: 45h

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- 1. J. Huheey, Inorganic Chemistry, Harper and Collins, NY IV Edition, 1983.
- 2. H.J. Arnikar, Nuclear Chemistry, Wiley Eastern Co. II Edition, 1987.
- F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry- A Comprehensive Text, John Wiley and Sons, V Edition, 1998.

- 1. K. F. Purcell and J.C. Kotz, Inorganic Chemistry-WB Saunders Co., USA,
- 2. M.C. Day and J. Selbin, Theoretical Inorganic Chemistry, Van Nostrand Co., New York, 1974.
- 3. D.F. Shrivers, P.W. Atkins and C.H. Langfor, Inorganic Chemistry, Freeman, New York, 1990.

To study the general aspects of alkaloids, steroids, camphor, squalene, Acetic acid, carbohydrates and polysaccharids.

UNIT – I Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis of the following: Ephedrine, Atropine, Quinine and Morphine.

UNIT – II Steroids-I

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon, stereochemistry, isolation, structure determination and interconversions of steroids.

UNIT – III Steroids-II

Bile acids, Androsterone, Testosterone, Estrone, Progestrone, Aldosterone and bio synthesis of cholesterol

UNIT – IV Terpenoids

Terpenoids-Classification, Isoprene rule, Structural elucidation by chemical degradation and synthesis of camphor, Squalene, and Abetic acid.

UNIT – V Carbohydrates

Carbohydrates –Oligosaccharides, trisaccharides glycosides. Structural Elucidation of Starch and cellulose, Primary concept.

Course Outcomes:

- To learn the general aspects of alkaloids in plants.
- To know the structure, stereochemistry and synthesis of quinine and morphine.
- To learn about the occurrence, nomenclature and basic skeleton of steroids.
- To elucidate the structure and interconversions of steroids.
- To understand the types of steroids.
- To familiarize the classification of terpenoids and synthesis of camphor.
- To know how to elucidate the structure of terpenoids by chemical degradation method.
- To understand how to elucidate the structure of starch and cellulose.

TEXT BOOKS:

- 1. R.O.C. Norman, Chapman and Hall, Principles of Organic Synthesis, London, 1980.
- 2. E.S. Gould, Structure and mechanism in Organic Chemistry, Henry Holt and Co. New York, 1957.

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TOTAL : 45h

- 3. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry-Part B, 3rd Edition, 1990.
- 4. S.M. Mukherji and S.P. Singh, Organic Reaction Mechanism, Macmillan India Ltd., 1990.

- 1. Michael.B.Smith, Organic Synthesis, Elsevier Inc, Third Edition, 2010.
- 2. Mc.Murray, Advanced organic chemistry, Thomson Pvt. Ltd., 1998.

> To study the anaesthetics, sedatives, hypnotics, analgesics, antibiotics, enzymes, coenzymes, vitamin and photo transfer catalysis.

UNIT – I **Classification of Drugs**

Classification of drugs- general and local anesthetics. Sedatives and hypnotics. Narcotics and analgesics.

UNIT – II Antibiotics

Antibiotics – structure and synthesis; Chloromphenicol, pencillins and streptomycin.

UNIT – III Enzymes

Enzymes, co enzymes, theory Enzymes structure - primary, secondary, tertiary and quaternary. Enzyme kinetics, Enzyme inhibitors, irreversible and reversible inhibitions, K_{cat} inhibitors. Transition – State analogues. Enzyme Inhibitors as drugs like cytochrome P450 inhibitors, Aromatase, lipoxygenases. Protein and peptide drugs - insulin, somatostatin, Relaxin, DNAse interferon, inteleukin, Growth stimulating factors and urokinase enzymes.

UNIT – IV Phase transfer catalysis

Phase transfer catalysis- principle, uses of crown ethers, ionic liquids and miscellaneous catalysts.

UNIT – V Vitamins

Vitamins – Introduction, water, fat soluble vitamins. Details of vitamin A, C, B₁, B₂ and B_6 .

Course Outcomes:

- To familiarize the basic classification of drugs. ٠
- To learn about the structure and synthesis of antibiotics. •
- To know the classification of enzymes. •
- To understand the protein and peptide drugs.
- To learn the principles of phase transfer catalysis. •
- To know about the uses of crown ethers. ٠
- To familiarize the water and fat soluble vitamins.
- To know the functions of vitamin A, C, B1, B2 and B6 in the body. ٠

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TOTAL: 45h

- 1. William O. Foye, Thomas L. Lemke, David A. Williams, Principles of Medicinal Chemistry, Lippincott Williams & Wilkins, 4th Edition, 1995.
- 2. Wilson & Gisvold's Textbook of Organic Pharmaceutical and Medicinal Chemistry, John.M. Beale and John. H. Block, Lippincott Williams & Wilkins,10th Edition, 1998.

- 1. M.E. Wolf, Burger's Medicinal Chemistry and Drug Discovery:Therapautic Agents, Wiley Blackwell; 5th Edition edition, 1997.
- 2. G.L. Patrick, "Introduction to medicinal chemistry", Oxford University Press, 1995

- > To under Nuclear fission and nuclear fusion, reaction and applications of tracers
- To study; the features of inorganic photochemistry like solar energy conversion and photo electrochemistry.

UNIT-I Electron Capture Detectors

Orbital electron capture: nuclear isomerism, internal conversion, detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M., Scintillation and Cherenkov counters.

UNIT-II Nuclear fission and fusion reactions

Nuclear fission and fusion reactions as energy sources: direct reactions, photonuclear and thermo nuclear reactions. Components of nuclear reactors – the breeder reactor – nuclear reactors in India.

UNIT-III Tracer study in Analytical Chemistry

Applications of tracer in study of reaction mechanism and in analytical chemistry – neutron activation analysis – isotope dilution analysis –Carbon dating- radio active tracer in the diagnosis and treatment in field of medicine.

UNIT-IV Photochemistry

Physical properties of electronically excited molecules – Dipole moment, pKa and redox potentials - Fluorescence, phosphorescence and delayed emission - Stern Volmer equation-Derivation, limitations and applications - Photosensitisation and chemiluminescence - Experimental techniques-

UNIT- V Photo redox reactions and Photo substitution reactions

Photo redox reactions and photo substitution reactions in coordination chemistry - photovoltaic and photo galvanic cells. Photo electro chemistry, Aspects of solar energy conversion.

Course Outcomes:

- To learn what is cloud chamber and bubble chamber.
- To know various reactions of nuclear fission and nuclear fusion.
- To familiarize the nuclear reactors in India.
- To apply tracer study in analytical chemistry.
- To learn how radioactive tracer is used in diagnosis and treatment in the field of medicine.
- To understand fluorescence, phosphorescence and delayed emission.
- To know what is photo voltaic and photo galvanic cells.

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TOTAL: 45h

• To learn the concepts of solar energy conversion.

TEXT BOOKS:

- 1. G.S. Manku, Inorganic Chemistry, TMG Co., 1984
- 2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry- A Comprehensive Text, John Wiley and Sons, V Edition, 1998.

- 1. D.F. Shrivers, P.W. Atkins and C.H. Langfor, Inorganic Chemistry, CH Langford, 1990
- 2. N.N. Greenwood and Earnshaw, Chemistry of the Elements, Pergamon Press New York, 1984.

CHEMICAL AND INSTRUMENTAL METHODS

OF DRUG ANALYSIS

Course Objective:

To understand the basic principles, instrumentation and applications in drug analysis using IR, UV-Visible, NMR and Mass spectrometry.

UNIT – I **UV-visible Spectrophotometry**

Theory – Beer Lambert's law – limitations of the law, Design and working of single beam and double beam spectrophotometry. Applications of UV absorption spectrometry in qualitative analysis and quantitative analysis.

UNIT-II **Differential Thermal Analysis**

Differential Thermal Analysis Differential Calorimetry. and Scanning Polymorphism/XRD – analysis.

UNIT-III **IR-Spectrometry**

Theory - Molecular vibration, instrumentation and mechanics of measurement sample preparation –IR Spectrometry,. FTIR and use in structural elucidation

UNIT – IV NMR Spectrometry

Theory, spin-spin coupling, chemical shift, magnetic equivalence – spin-spin decoupling - shift reagents instrumentation. Applications of NMR spectrometry in characterization of chemical structure using spectra of simple organic compound as examples. Principles, Instruments and applications of C¹³ NMR.

UNIT – V Mass Spectrometry

Theory, fragmentation pattern, ionization techniques; electron bombardment, chemical ionization, field desorption, fast atom bombardment. Different analysers, Interpretation of mass spectra, Determination of molecular weight and molecular formula and applications of mass spectrometry.

TOTAL: 45h

Course Outcomes:

- To familiarize the theory and working of single and double beam spectrophotometry.
- To apply the UV absorption spectrometry in analysis. •
- To know about differential thermal and scanning calorimetry.
- To elucidate the structure using FTIR technique.
- To apply NMR spectrometry in characterization of chemical structure using some • examples.
- To understand the applications of 13C NMR.

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- To know how to write fragmentation pattern of mass spectrometry.
- To understand what is molecular formula and molecular weight.

- Y.R.Sharma, Elementary Organic Absorption Spectroscopy, S.Chand & Co., 2nd edition New Delhi,1996.
- Robert M.Silverstein, Clayton Bassler and Terence C.Morril, Spectrophotometric Identification of Organic Compounds, 6th Edition, John Wiley & Sons, New York, 2002.

- 1. A. H. Beckett and J. B. Stenlake, Practical Pharmaceutical Chemistry Part-I and II, 4th Edition, CBS Publisher, Delhi,1998.
- H. H. Willard, L.L. Meritt, J. A. Dean and F. A. Settle, Instrumental Methods of Analysis, 7th edition, Wadsworth, New York, 1986.
- John R. Dyer, Applications of absorption spectroscopy of Organic Compounds, Prentice Hall, London, 1987.

SYNTHESIS OF ACTIVE PHARMACEUTICAL INGREDIENTS 3003 AND THEIR MANUFACTURE

Course Objective:

> To understand the process chemistry, combinatorial chemistry, phase transfer catalysis and asymmetric synthesis and strategy of process research.

UNIT – I Process Chemistry in Pharmaceutical Industry – An overview 09

Introduction, top 200 prescription drugs by worldwide sales ; Top ten drugs in the US market constituting 10% of world wide sales – Premarin, Synthroid, Lipitor, Prilosec, Hydrocone, Albuterol, Norvasc, Claritin, Timox and Prozac (\$ one billion). Background of process chemistry – role of process chemistry.

UNIT – II Strategy of Process Research & Development in Pharma Industry 09

Process research and development of PenicillinG CAS Reg.No.[61-33-6](antibacterial); fosinopril CAS Reg. No.[98048-97-6](antihypertensive) ; Rabeprazole CAS Reg. No.[117976-89-3] (antiulcerative) Time based competition – portfolio management – stages of process research and development.

UNIT – III Combinatorial chemistry

Introduction – Drug Optimization – Drug discovery – Solid Phase Technique – parallel synthesis – Mixed Combinatorial Synthesis – Deconvolution – Structure Determination and limitations – Drug design / Drug discovery.

UNIT– IV Phase transfer catalysis and Asymmetric synthesis 09

Application of phase transfer catalysts in pharmaceutical industry for drug synthesis – enantioselective synthesis of chiral 2-hydroxycarboxylic acids and esters – asymmetric catalysis – eg. Asymmetric hydrogenation – L-Dopa process; Sharpless asymmetric epoxidations eg. Synthesis of Fluoxetine enantiomers

UNIT –V Polymorphism and Process safety in Drug synthesis

Polymorphism – solid state – crystallization – recrystallization of drug molecules eg. Isolation techniques and characterization of polymorphs of Venlafaxine hydrochloride [99300-78-4] Clopidogrel bisulphate [135046-48-9] and Lorazepam[846-49-1] (any two) Chemical Process safety – Principles and Practice-guidelines and norms-Green chemistry.

TOTAL: 45h

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Course Outcomes:

- To familiarize about 200 prescription drugs by worldwide sales.
- To learn the background role of process chemistry.
- To familiarize the role of process research and development of pencillin G fosinopril and rabeprazole.
- To know the various stages of process research and development.
- To learn the drug discovery, drug design and optimization.
- To apply phase transfer catalysts in pharmaceutical industry for drug synthesis.
- To understand what is crystallization and recrystallization of drug molecules.
- To know the guidelines of green chemistry.

- 1. R. Hilfiker, Polymorphism in Pharmaceutical industry, Wiley-VCH, 2006.
- 2. H.G. Britain, Polymorphism in Pharmaceutical solids, CRC Press, Second edition, 1998.
- 3. Guidelines for safe process operations and maintenance, CCPS, John Wiley & Sons.
- 4. Guidelines for integrating Process safety management, environment, safety, health and quality, CCPS, Jon Wiley & Sons.

- Process Chemistry Eds M F Lipton, A G M Barrett & J Michl, Chemical Review 2006 V109 pp. 2581-3027.
- 2. The Merck Index, Merck & Co./ Inc. NJ USA,14th Edition,2006.
- 3. K G Gadamasetti, Process chemistry in Pharmaceutical industry Ed., Marcel dekker, Inc. NY USA, 1999.

ORGANOMETALLIC CHEMISTRY AND PHOTOCHEMISTRY 3003

Course Objective:

- > To know the bonding in some important organometallic compounds and their reactions.
- > To study some fundamental aspects of inorganic photochemistry.

UNIT – I Alkyls and Arene complexes

Alkyls and Arene complexes; metalation, bonding in metal carbonyls and nitrosyls, chain and cyclic donors, olefin, acetylene and allyl systems, synthesis, structure and bonding metallocenes.

UNIT – II Organometallic reactions

Organometallic reactions- Association, Carbonylation, decarbonylation, Insertion, Elimination and rearrangement.

UNIT – III Organometallic Catalysis

Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalysts (oxoprocess), oxidation of olefins to aldehydes and ketones (Wacker process).

UNIT-IV Polymerization

Polymerization (Zeigler-Natta catalyst); cyclo oligomerisation of acetylene using nickel catalyst (Reppes' catalyst)-Synthetic Gasoline-Mobil reaction.

UNIT – V Photo redox reactions and photo substitution reactions

Photo redox reactions and photo substitution reactions in coordination chemistry photovoltaic and photo galvanic cells. Photo electro chemistry, Aspects of solar energy conversion.

Course Outcomes:

- To learn the bonding in metal carbonyls and nitrosyls.
- To understand the synthesis, structure of metallocenes.
- To familiarize the various reactions of organometallic reactions.
- To know hydrogenation, hydroformylation and oxidation of olefins.
- To learn what is polymerization reactions.
- To understand synthetic gasoline.
- To know what is photovoltaic and photogalvanic cells.
- To learn the aspects of solar energy.

TEXT BOOKS:

1. J.E. Huheey, Inorganic Chemistry, Principles, Structure and Reactivity: Harper Collins, New York, fourth Edition, 1993.

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TOTAL: 45h

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2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry- A Comprehensive Text, John Wiley and Sons, fifth Edition, 1998.

- 1. K. F. Purcell and J.C. Kotz, Inorganic Chemistry, WB Saunders Co., USA, 1977.
- 2. Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller, Fraser Armstrong, Shriver and Atkins Inorganic Chemistry, Oxford University Press, New Delhi, fourth edition,2006.

> To understand the salient features of UV, visible, mass, infrared spectroscopy. To account of proton and ¹³C-NMR.

UNIT – I UV and Visible Spectroscopy

Introduction – the energy of excitation. The absorption laws, measurement of the spectrum – choice of solvent – selection rules and intensity – Chromospheres – solvent effects – Conjugated dienes, polyenes, ketones and aldehydes. $\pi - \pi^*$ transitions, n - π^* transition, ∞,β - unsaturated ketones, acids, esters, nitriles, amides. The benzene ring, the substituted benzene ring – polycyclic aromatic hydrocarbons the effect of steric hindrance to co planarity.

UNIT – II Mass spectroscopy

Introduction – Instrumentation – High resolution and low resolution mass spectra – Determination of molecular formula – Molecular peaks rule. M⁺ ion. Natural isotope abundance analysis – fragmentation process – nitrogen rule, metastable ions, metastable peaks, retro Diels – Alder fragmentation – McLafferty rearrangement, loss of odd electron, neutral fragments from molecular ions – Factors which influence fragment abundance – Mass spectra of various functional groups containing compounds to be studied: aromatic, aliphatic hydrocarbons, ketones, acids, esters, amides, ethers, alcohols, amine and nitriles.

UNIT – III Infrared spectra

Introduction – Preparation of samples and examination in an infrared spectrometer – The infrared spectrum – the use of the table of characteristic group frequencies – correlation charts. Absorption frequencies of triple bond and cumulative double bonds – the aromatic overtone and combination – Region 2000 – 1200 cm⁻¹. Absorption frequencies' of the double bond region – Groups absorbing in the finger print region – identification of functional groups.

UNIT – IV Proton carbon – 13 nuclear magnetic resonance

The spinning nucleus – The effect of an external magnetic field, precessional motion, precessional frequency, energy transitions. Theory of NMR – Measurement of chemical shifts – Internal standards – Units used in NMR. Factors influencing chemical shift – electronegativity, shielding and deshielding, Van der Walls deshielding, Anisotropic effects – Correlation data, use of correlation tables. Influence of restricted rotation. Chemically equivalent and magnetically equivalent protons. Solvents used in NMR – Choice of solvent – solvent shifts – concentration and temperature effects.

UNIT-V Splitting of signals in NMR and ¹³C-NMR

Integrals – Spin spin splitting – The splitting of NMR signals – Theory of spin-spin splitting. Magnitude of coupling, coupling constants. Proton exchange reactions. Factors influencing geminal coupling – vicinal coupling – Hetero annular coupling, Deuterium exchange. Improving the NMR spectrum – shift reagents. Effect of changing the magnetic field. Nuclear overhauser effect, spin tickling. Problems (Problems involving UV, IR and NMR to be solved) Carbon – 13 NMR: Principle, spin decoupled spectra, single frequency off resonance decoupled (SFORD) spectra, chemical shift values, problems.

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Course Outcomes:

- To learn the salient features of UV and Visible spectroscopy.
- To know about the instrumentation of mass spectroscopy.
- To understand what molecular peaks rule and fragmentation pattern.
- To identify characteristic group frequencies and functional groups in IR spectra.
- To know the theory of NMR like chemical shift and internal standard used.
- To learn the solvents used in NMR and choice of solvent.
- To understand the splitting of NMR signals and C13 NMR.
- To solve the problems related to UV, IR and NMR.

TEXT BOOKS:

- 1. Robert M. Silverstein, Clayton Bassler and Terence C. Morril, Spectrophotometer Identification of Organic Compounds, 6th Edition, John Wiley & Sons, New York, 2002
- 2. Donald L.Pavia, Gary M.L.Lampman, George S. Kriz, James R. Vyvyan, Spectroscopy, Cengage Learning India Private Ltd., 2007.

- 1. H. H. Willard, L. L. Meritt, J. A. Dean and F. A. Settle, Instrumental Methods of Analysis, Wadsworth, New York, 7th edition, 1986.
- John R. Dyer, Applications of absorption spectroscopy of Organic Compounds, Prentice Hall, London, 1987.

> To learn about the basic concept of stereochemistry of organic compounds. To learn about coupling reactions, retro synthesis analysis, and green chemistry.

UNIT – I Stereochemistry

UNIT – II Coupling Reactions

Stereochemistry: a) General consideration of molecular asymmetry and dissymmetry. Configuration – absolute and relative methods of determination, Chemical transformation, asymmetric synthesis.

Chiral auxiliaries, chiral reagents and catalysts, Enantiomeric excess, Quasiracemates Atropisomerism of biphenyls. Coupling reactions – Hock coupling – Suzuki coupling – Tin coupling – Transaction metal catalyses coupling reaction.

UNIT – III Retrosynthetic Analysis-I

Basic principles and terminology of retro synthesis, synthesis of aromatic compounds, one group C-C and two group C-C disconnection.

UNIT – IV Retrosynthetic Analysis-II

Retro-synthetic approach of Amine and alkene synthesis, Robinson annulations, Micheal addition and important functional group interconversions.

UNIT – V Synthetic Methodology

Protection, of functional groups (hydroxyl, amino, carboxyl, and carbonyl groups, Terminal alkyne). Illustration of protection and deprotection in synthesis

TOTAL: 45 h

Course Outcomes:

- To learn the molecular asymmetry and dissymmetry of stereochemistry. ٠
- To know about the absolute and relative methods of determination. •
- To understand what is chiral auxiliaries, chiral reagents and catalysts.
- To familiarize the various coupling reactions.
- To know the basic principles and terminology of retro synthesis.
- To learn the important strategies of ret rosy group transposition.
- To understand the important functional group interconversions •
- To know about the concept of green chemist •

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- 1. P. S. Kalsi, Stereochemistry Conformation and Mechanism, New Age International Publication, 2005.
- 2. Eliel, Stereochemistry of Carbon Compounds, Tata Mc Grawhill Education, 1975.
- 3. E.S. Gould, Mechanism & structure in organic Chemistry, Holt, Rinehart & Winston, New Delhi,1963.

- 1. Morrison and Boyd, Organic Chemistry, Pearson Education Inc, Sixth Edition, 1992.
- 2. I.L. Finar, Organic Chemistry, Longmans Green & Co., Third Edition, 1964.

NOVEL MATERIALS AND GREEN INDUSTRIAL 3 0 0 3 CATALYSIS

Course Objective:

> To know about nanomaterials, supported metallic clusters, metal oxides, supported metal oxides and environmental catalyst.

UNIT-I Introduction to Functional and Nanomaterials

An overview-, materials, molecular materials, functional materials, nanomaterial's classification /properties and industrial applications.

UNIT- II Properties of Metallic clusters

Supported metallic clusters, Catalysts preparation method, physical and chemical properties.

UNIT- III Characterization

Tools for Structural Characterization of novel materials-IR, NMR, Mass, ESR, Raman,

SEM and TEM

UNIT- IV Metal Oxides

Metal oxides, Supported metal oxides, Industrial catalysis (Synthesis Gas and

Hydrogen).

UNIT-V Catalysts in chemical transformation

Ammonia Synthesis, Methanol and Fischer – Tropsch Synthesis, Hydrocarbon Transformations, Environmental Catalysis

Course Outcomes:

- To overview the functional and nanomaterial.
- To know about the classification and industrial applications of nanomaterial.
- To familiarize the preparation and properties of metallic clusters.
- To understand the tools used for structural characterization of novel materials.
- To know the metal and supported metal oxides.
- To learn the use of industrial catalysts.
- To familiarize the catalysts in chemical transformation.
- To know about the environmental catalysis.

TEXT BOOKS:

1. Harry R. Allcock, Introduction to Materials Chemistry, Wiley Interscience Publisher.

TOTAL: 45h

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2. Bradley D. Fahlman, Materials Chemistry, 2nd edition, Springer Publisher, 2011.

REFERENCE BOOK:

1. Paul T. Anastas, Tracy C. Williamson, Green Chemistry: Frontiers in Benign Chemical Syntheses and Processes, Oxford University Press, 1998

- To understand the electrolytic conductance and the electrode and mechanism of electrode reaction.
- > To know about the general salient features of group theory.

UNIT-I Electro Chemistry-I

Mean ionic activity and mean ionic activity coefficient – concepts ionic strength. Nernst equation- redox system- electrochemical cell- Electrolytic conductance- Kohlraush's law and its applications, ionic equilibria. Debye- Huckel theory of strong electrolytes – Determination of activity coefficient by electrical method –Debye-Huckel limiting law qualitative and quantitative verification – Limitation of Debye –Huckel theory at appreciable concentration – Huckel equation – Debye- Huckel –Bronsted equation.

UNIT-II Electro Chemistry-II

Electrode –electrolyte interface – adsorption at electrified interface- electrical double layer – Electrocapillary phenomenon – Lippmann Equation – Structure of double layers – Helmholtz – Perrin- Guoy-Chapman and Stern model of electrical double layers. Mechanism of electrode reaction – Polarisation and overpotential – the Butler Volmer equation for one step and multi-step electron transfer reaction – Significance of exchange current density and symmetric factor-transfer coefficient and its significance – Mechanism of the hydrogen and oxygen evolution reactions.

UNIT-III Group Theory- I

Symmetry elements and symmetry operations – Mathematical rules for the formation of a group- Definition and classification of Point groups – Identification and determination – Matrix representations- Reducible and irreducible representations- Similarity transformation - Orthogonality theorem and its consequences.

UNIT-IV Group theory-II

Character table- Construction of Character table for C_{2V} and C_{3V} point group. Determination of symmetry of hybrid orbitals-Symmetry of hybrid orbitals in non linear molecules (H₂O, CH₄, XeF₄, BF₃, SF₆ and NH₃).

UNIT-V Group theory-III

Molecular vibrations -Direct product representation-Determination – IR and Raman activity of vibrational modes in non linear molecules (H_2O , CH_4 , XeF_4 , BF_3 , SF_6 and NH_3). Mutual exclusion principle. Symmetry selection rules of infrared and Raman Spectra. Selection rules for electronic transitions. Symmetry of molecular orbitals and electronic states of HCHO. Selection rules for electronic transitions of HCHO.

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Course Outcomes:

- To learn the electrochemical cell and electrolytic conductance.
- To determine the activity coefficient by electrical method.
- To understand the mechanism of electrode reaction.
- To know about the mechanism of hydrogen and oxygen evolution reactions.
- To define and classify the point groups.

TEXT BOOKS:

- Ramakrishnan and M.S Gopinathan, Group Theory in Chemistry, Vishal Publishing Co., 1988.
- 2. K.V.Raman, Group theory and its applications to Chemistry, Tata McGrowHill, 1990.

- 1. J. O. M.Bokris & A.K.N.Reddy, Electrochemistry, Plenum, New York, Vol 1 & 2, 1997.
- 2. P. Delahay, Electrode kinetics & Structure of double layer, Interscience, New York, 1965.
- 3. Robbins, Ions in solution, An introduction in electrochemistry, Clarendon press, Oxford, 1993.

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Course Objective:

- > To understand the bonding in polyacids, polymers and boronhydrides.
- > To study the complexes with references to bonding, stability and stereo chemistry.

UNIT -I Bonding In Inorganic Compounds –I

Poly acids: Isopolyacids and heteropolyacids of vanadium, chromium, molybdenum and tungsten. Inorganic Polymers: Polysilanes and Silicones.Poly sulphur – nitrogen compounds.

UNIT- II Bonding In Inorganic Compounds –II

Boron hydrides: Polyhedral boranes, carboranes and metallo carboranes.Metal Clusters: binuclear compounds, multiple metal-metal bonds.

UNIT – III Coordination Chemistry-I

Stability of complexes; thermodynamic aspects of complex formation; factors affecting stability; HSAB approach.Determination of stability constants by spectrophotometric, polarographic and potentiometric methods.

UNIT- IV Coordination Chemistry- II

Stereochemical aspects; Stereoisomerism in inorganic complexes, isomerism arising out of ligand and ligand conformation; chirality and nomenclature of chiral complexes; optical rotatory dispersion and circular dichroism.

UNIT- V Theories of Coordination

Crystal field theory and its limitations, d-orbital splitings, LFSE, spectro chemical series, evidences for metal ligand orbital overlap, molecular orbital theory - octahedral complex with σ and π bonding, John-Teller distortion, charge-transfer spectroscopy.

TOTAL: 45h

Course Outcomes:

- To know the structure and bonding in molecules / ions and predict the structure of molecules / ions.
- To learn the periodic properties of the different groups of compounds focusing on production methods and application of selected elements and compounds.
- 1To know the different definitions of acids / bases and predict the reactions between acids and bases.
- To learn the selected crystal structures and to explain what kind of parameters that affect the crystal structure of a compound

- 1. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Co., 1977.
- 2. J. Huheey, Inorganic Chemistry, Harper and Collins, New York, IV Edition, 1983.

- 1. R. B. Jordan, Reaction Mechanism of inorganic and Organometallic Systems, Oxford University Press, Third edition, 1991.
- 2. F.A. Cotton, F.A. Hart, The Heavy Transition Elements, McMillan Co., 1975.

- > To study the metabolism of carbohydrates, aminoacids, proteins and lipids.
- > To understand the functions of DNA and RNA.
- > To know about vitamins.

UNIT-I Chemistry and Metabolism of Carbohydrates

Definition, Classification and biological role of carbohydrates. Monosaccharides Linear and ring structures (Haworth formula) of ribose, glucose, fructose and mannose (structural determination not required) physical and chemical properties of glucose and fructose.

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

UNIT – II Chemistry and Metabolism of Amino acids and Proteins

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

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

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

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

UNIT - III Chemistry and Metabolism of lipids

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

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

UNIT- IV Nucleic Acids

Purine and pyrimidine bases, nucleosides, nucleotides, polynucleotides, DNA structure – various types, RNA structure – various types.

Biological functions of DNA and RNA, Genetic code.

UNIT- V Vitamins

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

Course Outcomes:

- To define, classify and biological role of carbohydrates.
- To know about the glycolysis of carbohydrates.
- To learn the essentials of amino acids in biology.
- To familiarize the biological functions of proteins.
- To understand the various types of lipids along with their properties.

TOTAL : 45h

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TEXT BOOKS:

- 1. G.R. Agarwal and O. P. Agarwal, "Text book of Biochemistry", Goel publishing House, 1984.
- 2. L. Styrer, "Biochemistry", Free man & Co., New York, 1994.

- 1. R.K. Murray, P.A., Mayes, D.K. Granner and V.W. Rodwell, "Harper's Biochemistry" (Lange Medical Book), 1990
- 2. B.L. William and K. Wilson, "Principles and Techniques of practical Biochemistry", Edward Arnold, London, 1990.

ORGANIC NAME REACTIONS AND SYNTHESIS 4004 OF REAGENTS

Course Objective:

To study condensation reaction oxidation and reduction reaction. To know the synthesis and application of important reagent.

UNIT-I **Organic Reactions - I**

Condensation reactions of the following; Aldol, Claisen ester condensations. Cannizzaro reaction, Dieckmann cyclisation, Reformatsky reaction, Dakin reaction, Etard reaction, HVZ reaction, Umpolung synthesis and Stephen reaction.

UNIT-II **Organic Reactions – Oxidations**

Barton reaction, Jones oxidation, Oppenauer oxidation and Michel addition.

UNIT-III **Organic Reactions – Reductions** 12

Birch reduction, Clemmenson reduction, Meerwin P.V reduction, rosenmund reduction.

UNIT-IV **Organic Reagents-I**

Synthesis and applications of the following reagents: 9-BBN, n-butyl lithium, ceric ammonium nitrate(CAN), DCC, Grignard reagent, LDA, Gilman reagent, NBS and PCC.

UNIT-V Organic Reagents- II

Use of the following reagents in organic synthesis and functional group transformations- complex metal hydrides, Hilmans reagent, lithium dimethyl cuprate,, dicyclohexyl carbodimide,1,3-dithiane, woodward and provost hydroxylation, selenium dioxide, crown ethers and Peterson's synthesis, Wilkinson's catalyst, Baker yeast.

TOTAL: 60h

Course Outcomes:

- To learn what is condensation reactions.
- To familiarize the various condensation reactions.
- To know the organic reactions of oxidations.
- To know the organic reactions of reductions.
- To understand how to synthesize some reagents.

TEXT BOOKS:

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- 1. R.O.C. Norman, Principles of Organic Synthesis, Chapman and Hall, London, 1980.
- 2. Francis A. Carey, Richard J. Sundberg, Advanced Organic Chemistry-Part B,3rd Edition 1990.
- 3. S.M. Mukherji, S.P. Singh, Organic Reaction Mechanism, Macmillan India Ltd. 1990.

REFERENCE BOOKS:

- 1. F.A. Cary, Organic Chemistry, Second edition, McGraw Hill, Inc., 1992.
- 2. P.S. Kalsi, Stereochemistry, Wiley Eastern Limited, New Delhi, 1990.

PHARMACEUTICAL FORMULATION TECHNOLOGY 4004

> To understand physicochemical principles, pharmaceutical operation and profile formulation.

UNIT-I Introduction

Need for formulation; History of formulation; Challenges in early formulations; Drug substance to Drug product with reference to formulating for the patient; Physical and chemical properties of Formulation.

UNIT-II **Physicochemical Principles**

Solutions ; pH, EMF and redox potentials ; physicochemical properties evolving into in vivo bioavailability; Absorption, Dissolution, Permeability, Distribution, Metabolism, Excretion; Complexation,; Modifies release dosage forms; profile of common formulations; colloidal systems, Rheology; Drug stability and ICH Guidelines for stability testing.

UNIT-III **Pharmaceutical Operations-I**

Extraction; Drying ; Evaporation; Distillation; Filtration/Centrifugatio; Size reduction and handling of solids in the powder form.

UNIT- IV **Pharmaceutical Operations-II** 12

Antisolvent and reactive crystallization; Melting approaches to particle size; Wet milling and dry milling; packaging.

UNIT-V **Profile of Formulations**

Tablets, capsules, solution and suspension formulation; Modified release formulation; Parenteral Formulation; Inhaled formulations/aerosols.

Course Outcomes:

- To learn the need, history and challenges in early formulations.
- To know what is drug substance to drug product with reference to formulating.
- To familiarize the various physicochemical properties evolving in bioavailability.
- To view the profile of common formulations.
- To know the ICH guidelines for stability testing.

TEXT BOOKS:

1. H. Mollet, H. A. Grubenmann, Pharmaceutical Technology, in Formulation Technology: Emulsions, Suspensions, Solid Forms, Wiley-VCH Verlag GmbH, Weinheim, Germany,2007.

TOTAL: 60h

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2. Mark Gibson, Drug Preformulation and formulation, Informa, New York, Second Edition, 2007.

Luition, 2007

- 1. S. K. Jain and V. Soni, Bentley's Textbook of Pharmaceutics-An Adaptation, Elsevier, 2012
- 2. C. B. Gupta and S. S. Khanka, Entrepreneurship and Small Business Management, Sultan Chand & Sons, New Delhi, 2013.

ENZYME TECHNOLOGY AND RELATED ENTEREPRENEURIAL SKILLS

Course Objective:

> To learn biological aspects, metelloenzyms, oxygen carriers, nitrogen fixation, photosynthesis and cytochrome, and bioanalytical aspects.

UNIT – I Basic concepts of Bioinorganic Chemistry

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

UNIT – II Enzymes

Essential and trace metal ions.Coenzymes – Vitamin B coenzymes, carboxy peptidase and Superoxide dismutase.

Heme – enzyme – Peroxidase and catalases.

UNIT – III Heme Proteins

Oxygen carriers – Hemeproteins – Hemoglobin, myoglobin – Structure Oxygenation and Stereochemistry – Bohr effect. Non-heme oxygen carriers – Hemerythrin and hemocyanin-Iron storage and transport proteins.

UNIT – IV Nitrogen fixation and biological redox reactions

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

Iron - sulphur proteins - rubredoxin and ferredoxin. Photosynthesis and chlorophyll's.

UNIT – V Bio analytical Chemistry

Bio analytical Chemistry, Toxicity & medicine, Toxicity of Hg, Cd, Zn, Pb, As, Sb, Anti cancer agents, Metal ion poisoning: Failure of metal ion control systems, role of metal ion

Diagnosis and treatment – use of radio isotopes,Pollution studies: Effluents and treatment. Inorganic plant nutrition and indicator plants for mineral exploration.

Course Outcomes:

- To learn the basic concepts of structure and functionality of thermodynamics and biology.
- To understand the various aspects of electrochemical phenomena.
- To familiarize the role of essential and trace metal ions in human body.
- To know the concepts of coenzymes, carboxy peptidase and superoxide dismutase.

79

• To learn the role of hemoglobin and myoglobin functions in human body.

TEXT BOOKS:

- 1. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Co., 1977.
- 2. G. N. Mugherjee, Arabinda Das, Elements of Bioinorganic Chemistry, 1993.

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TOTAL: 60h

3. M. Satake and Y.Mido, "Bioinorganic Chemistry", Discovery Publishing House, New Delhi,1996.

REFERENCE BOOK:

1. G. Eichron, Inorganic Bio-chemistry Vol. I and II, Elsevier, 1973.

To understand, electrocyclic reaction, sigma tropic rearrangement, photochemistry synthon, robinson ambulation, synthesis of carbene.

UNIT – I Electro cyclic reactions

Electro cyclic reactions - definition, classification, M.O treatment, FMO- PMO correlation diagram treatment with example. Application of electro cyclic reactions in organic synthesis. Cyclo addition reactions – classification – definition.

UNIT – II Sigma topic rearrangement

Sigma topic rearrangement – Hydrogen migration [1,3],[1,5]&[1,7] definition, classification, FMO-PMO treatment and correlation diagram. Hydrogen migration in cyclic system like cyclopentadiene, Indene cyclohepta trienes. Sigma topic rearrangement involving methyl group and chiral groups. Sigmatopic rearrangements in cope & Claisen reactions – FMO&PMO treatment. Degenerates molecules, Fluxional molecules, application of sigma topic rearrangement in organic synthesis.

UNIT – III Photo chemistry

Photo chemistry – Introduction to photochemistry, quantum yield cyclisation reaction and ring opening of 1, 3 Butadiene, 1, 3, 5 hexatriene systems. Primary & Secondary, photochemical reactions, photochemistry of carbonyl, Diene and Dienones.

UNIT – IV **Retrosynthetic Analysis**

Synthon, C-C, C = C bond formation by various method. (Aldol, Michael, Peterson, Shapiro, Wittig, Benzoin, Robinson annulations, Deick Mann condensation. Synthesis of enamines and their applications.

UNIT – V **Reagents in Organic Synthesis**

Reagents in organic synthesis: metal hydrides, Lithium dimethyl cuprates, LDA, 1, 3 dithione, trimethyl silyl iodide, 9BBN, DCC. Synthesis of cubane, 5- hexenoic acid, Bicyclo [4, 1, 0] heptanes -2-one.

Course Outcomes:

- To understand the definition, classification, applications and example of M.O, FMO and PMO.
- To know the classification and definition of cycloaddition reactions.
- To learn what is sigma topic rearrangement with definition and classification.
- To familiarize the various sigma topic rearrangement involving methyl, chiral, cope and claisen reactions along with their applications.
- To introduce the concept of photochemistry in organic chemistry.

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TOTAL: 60h

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4004

TEXT BOOKS:

- 1. R.O.C. Norman, Chapman and Hall, "Principles of Organic Synthesis" London, 1980.
- Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry-Part B", 3rdEdition1990.
- 3. S.M. Mukherji and S.P. Singh, "Organic Reaction Mechanism", Macmillan India Ltd.,1990.

- 1. Micheal Smith, Organic synthesis, Elsevier Inc, third edition, 1946.
- 2. Mc. Murray, Advanced Organic Chemistry, Thomson Pvt. Ltd, 1980.

STRATEGIC MANAGEMENT OF PHARMA 4004 INDUSTRY

Course Objective:

> To know about pharma industry, technology opportunity for innovation, project evaluation, intellectual property protective and business strategy.

UNIT I Introduction and Technology Evolution

Pharma industry-Specifics, Importance and role in health sector; the Global scenario and Positioning of Indian Pharma industry; Specific challenges of the Pharma industry versus the general industrial matrix; Understanding technological change; Need for technology strategy as step towards innovation and competitive advantage; Defining technological innovation and benefits.

Technology S- curves and management; Number of firms in the industry, Process obsolescence and Reverse Engineering; Innovative synthetic routes and atom economy dovetailing aspects of Green chemistry; Technology adoption and diffusion; Forecasting demand and confronting substitution.

UNIT II **Opportunity for Innovation**

Technological, Political and Regulatory changes, Diversification, Demographic changes; Research and Development (R&D); Investment in R&D and return on investment – a profit centre; Linking of Research and Development for leverage; Cost reduction exercises.

UNIT III **Project evaluation**

Managing uncertainty, Analytical hierarchy process, Net Present Value(NPV), Internal Rate of Return(IRR), scenario analysis and decision tree; Portfolio Management, customerfriendly solutions; Product pricing ; Market segmentation and market research.

UNIT IV **Intellectual Property Protection**

Role of IP protection in knowledge era; Patents- process and Product and the patenting process; Lead molecule development and cost; ANDA; Patent litigation; Nondisclosure agreement; Expiry of patents and generic drugs marketing and issues in IP.

UNIT V **Business strategy**

Networking; Joint venturing; Licensing; Contract manufacturing; Outsourcing; Human resource management of technical professionals- R&D personnel, Product Development team, Cross-Functional team, Internal communication, Organization structure- decentralizing R&D, acquisitions.

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Course Outcomes:

- To know the various pharma industry and their role in health sector.
- To understand technological change, innovation and benefits.
- To learn the evolution in technology.
- To understand how to invest in R and D and its return on investment.
- To familiarize the evaluation of project.

TEXT BOOKS:

- 1. Technology Strategy For Managers And Entrepreneurs-Scott Shane, Ind .ed. Dorling Kindersley India Pvt. Ltd. , 2009.
- 2. Entrepreneurship and Small Business Management-C.B.Gupta and S.S.Khanka, Sultan Chand & Sons, New Delhi, 2012.

REFERENCE BOOK:

 Jean Michel Peny, Pharma Market insight and strategy, Smart Pharma Consulting, First edition, 2013.

Syllabus

Generic Elective Courses

The ability to create an open environment for communication. An understanding of other people communication styles and needs. To create an environment for open discussion and ongoing dialogue is crucial for communication success.

Unit I Reading Comprehension and Vocabulary

Definitions of reading – types of reading – oral reading – silent reading – reading process – classification of reading – nature of reading – Filling in the blanks – Cloze Exercises – Vocabulary building – Reading and answering question.

Unit II Listening and Answering Question

Listening process – speaker – hearer – types of listening – transitional listening – critical listening – recreational listening – listening for appreciation – selective listening – intensive listening- extensive listening – listening and sequencing sentences – filling in the blanks – listening and answering questions.

Unit III Group Discussion

Introduction – Why GD Part of a selection process – Structure of a GD-Strategies in GD – Team work – body language – Debating various points of views – interaction with peers.

Unit IV Conversations

Introducing oneself and others, narrating events – making telephonic conversation – Giving instruction – Giving instruction- Expressing purposes and functions- obligation and preferences, Accepting offers and Counseling Face to face Conversations

Unit V Self – Introduction and Role Play

Introduction self and greetings- asking for information- offerings- requisitions- inviting – vocabulary building- asking for description.

Course Outcomes:

- Cloze exercises provide support to build vocabulary
- Sense of logic develops from sequencing sentences
- Group discussion infuses team spirit and sense of competition
- Face to face and telephone conversation builds up self confidence
- Self introduction and role play facilitate cultivation firmness of mind and empathy

TEXT BOOKS:

- 1. Barun K. Mitra, "Personality Development and Soft Skills". Oxford University Press. New Delhi. 2011.
- 2. S.P. Sharma, "Personalilty Development", Pustaq Mahal. New Delhi. 2010.

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TOTAL: 45 h

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1022

- 1. Meenakshi Raman and Sangeetha Sharma, "Technical Communication", Oxford University Press. New Delhi, 2009.
- 2. A.S. Hornby: "Oxford Advanced Learner's Dictionary of Current English", Oxford University Press, 2007

To provide basic information about presentation skill and train the students for letter writing, creation of resume and develop the interview skills. To provide information about the Process, types and patterns of communication.

Unit I **Presentation Skills**

General presentation methods and developing presentation skill

Unit II Soft skills (Time Management, Stress Management and Body Language) 09

Time management: Importance, Plan and Execution, Default reason and rectification methods. Stress Management: Stress Impacts over Efficiency and how to manage. Body Language: Its importance and need

Unit III **Resume / Report / Letter Writing**

Resume: Basic components of a resume, Preparation of a resume, Types of resume Report: How to prepare reports, reports components and structure Letter writing: types of letters, framing letters, basic structure, how to draft a letter

Unit IV **Frequently asked Questions**

Unit V Interview Skills

Aims of Interview expectations and how to fulfill, developing skills

TOTAL: 45 h

Course Outcomes:

- Self introduction and role play facilitate cultivation firmness of mind and empathy
- Group discussion infuses team spirit and sense of competition
- Listening regenerates transformation empathetically
- Cloze exercises provide support to build vocabulary
- Implementation of assertive thoughts can be acquired through writing skills

TEXT BOOKS:

- Barun K. Mitra, "Personality Development and Soft Skills". Oxford University Press. New 1. Delhi. 2011.
- 2. S.P. Sharma, "Personalilty Development", Pustaq Mahal. New Delhi. 2010.

REFERENCE BOOKS:

1. Meenakshi Raman and Sangeetha Sharma, "Technical Communication", Oxford University Press. New Delhi, 2009.

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2. A.S. Hornby: "Oxford Advanced Learner's Dictionary of Current English" Oxford University Press, 2007

- \geq To train the students to use eco-friendly approaches in synthesizing agro-based chemicals viz. insecticides, fungicides, herbicides, bactericides acaricides, weedicides
- \geq To emphasize green chemistry approach in crop protection which help to reduce global warming.

UNIT- I Introduction

Current status of chemistry and the Environment-Evolution of the Environmental movement: Public awareness - Dilution is the solution to pollution-Pollution prevention

UNIT-II Green Chemistry

Definition – Principles of Green Chemistry - Why is this new area of Chemistry getting to much attention - Why should chemist pursue the Goals of Green Chemistry - The roots of innovation Limitations

UNIT- III **Green Chemistry using Bio Catalytic Reactions**

Introduction - Fermentation and Bio transformations - Production of Bulk and fine chemicals by microbial fermentation- Antibiotics - Vitamins - Bio catalyses synthesis of industrial chemicals by bacterial constructs - Future Tends.

UNIT-IV **Green House Effect and Global Warming**

Introduction - How the green house effect is produced - Major sources of green house gases -Emissions of CO2 - Impact of green house effect on global climate - Control and remedial measures of green house effect - Global warming a serious threat - Important points

UNIT-V **Future Trends in Green Chemistry**

Green analytical methods, Redox reagents, Green catalysts; Green nano-synthesis, Green polymer chemistry, Exploring nature, Biomimetic, Proliferation of solvent-less reactions; Noncovalent derivatization, Biomass conversion, emission control.

TOTAL: 30h

Course Outcomes:

- To understand the connection between common atoms and complex molecules
- To explain and analysing simple chemical reactions
- To distinguishing between recyclable and non-recyclable materials
- To assessing the potential impact of chemical reactions to environment and human health
- To understand the connection at the chemical level between all matter and will develop your inquiry based activities to explore best practices related to organic farming and resource management.
- To about the advance technology in green chemistry

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TEXT BOOKS:

- 1. M. Lancaster, "Green Chemistry: an Introductory Text", RSC, 2002
- 2. Sheldon, Arends, Hanefeld, "Green Chemistry and Catalysis", Wiley, New York, 2007.

- 1. Anastas & Warner, Green Chemistry : Theory & Practice ,Oxford Univ. Press,New York, 1998.
- 2. S. E. Park, J. S. Chang, S. H. Jhung, "The Role of Catalyst for Green Chemistry", Chemworld, Vol. 44 (8), 38, 2004.

CHEMINFORMATICS

Course Objective:

- \geq Students completing this paper should be able to understand concepts of molecular chemistry that are basic to cheminformatics.
- This course will train the students to use QSAR, docking etc. \geq

UNIT- I Mathematics Process

Graph theory and molecular numerology; Logic, sets and functions; Algorithms, integers and matrices; Mathematical reasoning, induction and recursion; Counting; graphs, trees and sets, basic probability and statistics; Markov processes

UNIT- II **Basics of Stereochemistry**

Basic Stereochemistry, Amino acids and Proteins and Properties; pKa, pH and ionization of acids and bases; Protein structure - Primary structure, Secondary structure - helix & sheet; Tertiary structure; Quaternary structure; covalent and non-covalent forces that maintain structures.

UNIT- III **Chem Information**

History of scientific information communication-chemical literature-chemical informationchemical information search-chemical information sources-chemical name and formula searching-analytical chemistry-chemical history-biography-directories and industry sources

UNIT- IV **Biological Databases**

Introduction; Experimental sources of biological data; Publicly available databases; Gene expression monitoring; Genomics and Proteomics; Metabolomics; Visualisation of sequence data; Visualization of structures using Rasmol or SPDB Viewer or CHIME; Genetic basis of disease; Personalised medicine and gene-based diagnostics.

UNIT- V Drug Design

Introduction to drugs, structure-based drug design. QSAR and 3D-QSAR Methods. Pharmacophore Design, Ligand-Based Design and De Novo Drug Design Virtual screening/docking of ligands. Protein structure, Drug action & enzymes. Drug action & receptors. Prediction of Binding Modes, Protein-Ligand binding free energies, Fragment-Based Drug Design, ADMET prediction.

TOTAL: 30 h

Course Outcome:

- To understand basis of group theory and its applications
- To study Logics, sets and functions
- To get a clear idea on the principles and theories of algorithms, induction Basics and process of photosynthesis
- To understand the Basics of stereochemistry and structure of proteins
- To study History of science and chemical information
- To discuss the biological database and Gene expression

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2002

TEXT BOOKS:

- 1. P. Shanmughavel, "Principles of Bioinformatics", Pointer publishers, 2005.
- 2. Arfken, "Mathematical Methods for Physicists" Academic Press, 1985

- 1. P. Shanmughavel, "Trends in Bioinformatics", Pointer publishers, 2006.
- 2. Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry-Part A & B" Third Edition, 1990.

- \geq To understand the basic information of food chemistry and adulteration.
- \geq To appreciate the importance of food additives and pesticide control.
- \geq To provide an information about food preservatives

UNIT-I Introduction

Food: source, functions of food – food groups – food guide – basic five food groups, usage of the food guide – food in relation to health – objectives of cooking.

Water: Purification processes – Ion exchangers, reverse osmosis, activated charcoal treatment Use of chlorination, ozone, and UV light disinfection. Specification of drinking water.

UNIT-II **Constituents of Foods**

Carbohydrates: Classification, Principles involved in the analysis of carbohydrates –estimation of carbohydrates.

Proteins: amino acids – peptides - Analysis of proteins – Separation of amino acids by paper chromatography.

Minerals and vitamins: Sources, functions, deficiency of the following minerals (calcium, iron, iodine, fluorine, sodium and potassium (elementary treatment). Vitamins - classification, sources, Vitamins – A, D, E and K, C, B Complex, - B6 & B12.

UNIT-III **Food Additives**

Artificial sweeteners – saccharin, cyclomate, asparatame – food flavours – esters, aldehydes and heterocyclic compounds. Antioxidants. Food colours – changes in cooking..Restricted use. Spurious colours. Emulsifying agents, preservatives – leavening agents. Baking powder – Yeast. Taste enhancers – MSG-vinegar

UNIT-IV **Pesticides Control**

Spoilage of foods by insects and pests, loss in food quantity and quality Various pesticides used in agriculture and post-harvest storage, uses of pesticides for food grain application.

UNIT-V **Food Adulteration**

Common adulterants in different foods – milk and milk products, vegetable oils, and fats, spices and condiments, cereals, pulses, sweetening agents and beverages. Contamination with toxic chemicals – pesticides and insecticides. .

Course Outcomes:

- To know about the basic criteria of food and water standards for consumption
- To get a basic idea about the chemical constituents of food
- To learn about the various food additives, their chemical composition and their permissible level of usage in foods.
- To know about the various organisms which spoil the crops pre and post harvest and their control using pesticides

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TOTAL: 30h

• To know about the various food adulterants for different types of food and methods to detect those adulteration.

TEXT BOOKS:

- 1. Owen.R. Fennema, Food Chemistry, Marcel Decker Inc., New York. 1996.
- 2. M. Swaminathan, Text Book on Food chemistry, Printing and Publishing CO., Ltd., 1993.

- 1. B. Siva Sankar, Food Processing and Preservation, Prentice Hall of India Pvt. Ltd., New Delhi, 2002.
- 2. S. Ramakrishnan, K. G. Prasannam, R. Rajan, Principles Text book of medical biochemistry, Orient Longman Ltd., Third Edition, 2001.