MANAV RACHNA UNIVERSITY
FACULTY: FACULTY OF APPLIED SCIENCES
PROGRAM: M.Sc. CHEMISTRY
PROGRAM CODE: CHP01
SYLLABUS: SCHEME A

MANAV RACHNA UNIVERSITY
FACULTY OF APPLIED SCIENCES
DEPARTMENT OF CHEMISTRY
M.SC. (2017-2019)
SYLLABUS & SCHEME

(CHP01)
SEMSETER I

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core (Departmental/ Allied)/ Elective (Departmental/ Open) /University Compulsory	Hard/Soft/ Workshop/ NTCC	L	T	P	0		
CHH501	INORGANIC CHEMISTRY-I	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH502	ORGANIC CHEMISTRY-I	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH503	PHYSICAL CHEMISTRY-I	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH504	ANALYTICAL CHEMISTRY	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH505	LABORATORY WORK-I	CORE (Departmental)	HARD	0	0	8	0	8	4
CHW506	WORKSHOP	CORE (Departmental)	WORKSHOP	0	0	3	0	3	2
PHS-501	RESEARCH METHODOLOGY	CORE (Allied)	HARD	1	0	2	0	3	2

SEMESTER II

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core(Departmental/Allied)/ Elective (Departmental/ Open) / University Compulsory	Hard/Soft/ Workshop/ NTCC	L	T	P	O		
CHH508	INORGANIC CHEMISTRY-II	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH509	ORGANIC CHEMISTRY-II	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH510	PHYSICAL CHEMISTRY-II	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH511	SPECTROSCOPY	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH512	LABORATORY WORK-II	CORE (Departmental)	HARD	0	0	8	0	8	4
CHW513	WORKSHOP	CORE (Departmental)	WORKSHOP	0	0	3	0	3	2
MES 515	RESEARCH PAPER WRITING	CORE (Allied)	SOFT	1	0	2	0	3	2
CHW514	SUMMER TRAINING	-	-	-	-	-	-	-	3

Organic Chemistry Specialization
SEMSETER III

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core (Departmental/ Allied)/ Elective Departmental/ Open) / University Compulsory	Hard/Soft/ Workshop / NTCC	L	T	P	O		
CHH615	CONFORMATIONAL ANALYSIS, ASYMMETRIC SYNTHESIS & BIOMOLECULES	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH616	MODERN ORGANIC SYNTHESIS (REAGENTS & SYNTHETIC TECHNIQUES)	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH617 CHH618 CHH631	ELECTIVE-I A. BIOINORGANIC CHEMISTRY & ORGANOMETALLIC CHEMISTRY B. DRUG DESIGN C. POLYMER CHEMISTRY	CORE (Departmental)	ELECTIVE	4	0	0	0	4	4
CHH619	PHOTOCHEMISTRY & PERICYLIC REACTIONS	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH620	LABORATORY WORK-III	CORE (Departmental)	HARD	0	0	6	0	6	3
CHH621	LABORATORY WORK-IV – O	CORE (Departmental)	HARD	0	0	6	0	6	3
CHN622	SEMINAR	CORE (Departmental)		0	0	0	2	2	2

SEMSETER IV

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core (Departmental/ Allied)/ Elective (Departmental/ Open) / University Compulsory	Hard/Soft/ Workshop/ NTCC	L	T	P	O		
CHH623	ADVANCED HETEROCYCLIC CHEMISTRY	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH624	CHEMISTRY OF NATURAL PRODUCTS	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH625 CHH626	ELECTIVE-II (A) BIOORGANIC CHEMISTRY (B) GROUP THEORY AND ITS APPLICATIONS (C) NANOSCALE MATERIALS: SYNTHESIS, PROPERTIES AND APPLICATIONS	ELECTIVE (Departmental)	HARD	4	0	0	0	4	4
CHH627	LABORATORY WORK-V -O	CORE (Departmental)	HARD	0	0	6	0	6	3
CHN628	MAJOR PROJECT	CORE (Departmental)	NTCC	0	0	0	6	35	6

Inorganic Specialization
SEMSETER III

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core (Departmental/ Allied)/ Elective Departmental/ Open) / University Compulsory	Hard/ Soft/ Workshop/ NTCC	L	T	P	O		
CHH 629	INSTRUMENTATION TECHNIQUES AND SEPARATION METHODS	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH630	SOLID STATE CHEMISTRY	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH617 CHH618 CHH631	ELECTIVE-I A. BIOINORGANIC CHEMISTRY & ORGANOMETALLIC CHEMISTRY B. DRUG DESIGN C. POLYMER CHEMISTRY	CORE (Departmental)	ELECTIVE	4	0	0	0	4	4
CHH632	METAL CLUSTERS AND ADVANCED COORDINATION CHEMISTRY	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH620	LABORATORY WORK-III	CORE (Departmental)	HARD	0	0	6	0	6	3
CHH633	LABORATORY WORK-IV -I	CORE (Departmental)	HARD	0	0	6	0	6	3
CHN622	SEMINAR	CORE (Departmental)		0	0	0	2	2	2

SEMSETER IV

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core(Departmental/ Allied)/ Elective (Departmental/ Open) / University Compulsory	Hard/Soft/ Workshop/ NTCC	L	T	P	O		
CHH634	APPLIED ORGANOMETALLIC AND APPLIED BIO-CATALYSIS	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH635	NUCLEAR, RADIOCHEMISTRY AND LASERS	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH625 CHH626 CHH636	ELECTIVE-II (A) BIOORGANIC CHEMISTRY (B) GROUP THEORY AND ITS APPLICATIONS (C) NANOSCALE MATERIALS: SYNTHESIS, PROPERTIES AND APPLICATIONS	ELECTIVE (Departmental)	HARD	4	0	0	0	4	4
CHH627	LABORATORY WORK-V -I	CORE (Departmental)	HARD	0	0	6	0	6	3
CHN628	MAJOR PROJECT	CORE (Departmental)	NTCC	0	0	0	6	35	6

TOTAL CREDITS FOR SEMESTER I –IV

S. No.	Semester	Credits
1	I	24
2	II	24
3	SUMMER TRAINING (POST 2nd SEM)	3
4	III	24
5	IV	21
TOTAL CREDITS FOR M.Sc. CHEMISTRY PROGRAMME		96

SECTION WEIGHTAGE PARAMETERS

	Sections	Weightage
Syllabus	A	25%
	B	25%
	C	25%
	D	25%
	TOTAL	100%

SEMESTER I

DETAILED SYLLABUS
SEMESTER I

Course Title/Code	Inorganic Chemistry-I (CHH501)
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To familiarize students with Metal-Ligand Bonding in Transition Metal Complexes To impart knowledge on Electronic Spectra of Transition Metal Complexes
Outcome	The students will be able to understand ML bonding in transition metal complexes. The students will be able to understand electronic spectra of transition metal complexes. The students will be able to understand VSEPR and HSAB theory
Prerequisites	B.Sc. with Chemistry as one of the Subject

SECTION-A

METAL-LIGAND BONDING IN TRANSITION METAL COMPLEXES : Crystal field theory, Crystal field splitting diagrams in complexes; Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller distortions; experimental evidence for metal-ligand orbital overlap; ligand field theory, molecular orbital theory of octahedral complexes.

SECTION-B

ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES: Spectroscopic ground states; Orgel energy level and Tanabe-Sugano diagrams for transition metal complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral complexes and calculation of ligand-field parameters.

SECTION-C

VSEPR THEORY: Valence Shell Electron Pair Repulsion Theory – stereochemical rules and explanation of the shapes of molecules and ions of non-transition elements with 2-7 valence shell electron pairs, dπ -pπ bonds, Bent rule and energetic of hybridization

SECTION-D

HSAB Theory : Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardness and softness; Lewis-acid base reactivity approximation; donor and acceptor numbers, E and C equation; applications of HSAB concept.

Books Recommended

1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed. Pearson Education, 2006.
2. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.

3. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. Wiley, 1999.
4. R. C. Mehrotra and A. Singh, Organometallic Chemistry: A Unified Approach, New Age International, 2006.
5. A. J. Elias, B. D. Gupta; Basic Organometallic Chemistry: Concepts, Synthesis and Applications of Transition metals, CRC Press and Universities Press, 2010.
6. J. D. Lee; Concise Inorganic Chemistry, 4th ed. Chapman and Hall, 1991

Course Title	**Organic Chemistry-I (CHH502)**
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To familiarize students with aromaticity and Effects of Structure on Reactivity To impart knowledge of Nucleophilic Substitution and reactivity effects of substrate structure
Outcome	Students will be able to understand the concept of aromaticity and structure-reactivity correlation. Students will be able to grasp in depth knowledge of Nucleophilic and Electrophilic Substitution reactions.
Prerequisites	B.Sc. with Chemistry as one of the Subject

SECTION-A

AROMATICITY: Benzenoid and non-benzenoid systems, anti-aromaticity, homoaromaticity, alternant and non-alternant hydrocarbons. **EFFECTS OF STRUCTURE ON REACTIVITY:** Linear free energy relationships (LFER), the Hammett equation – substituent and reaction constants; the Taft treatment of polar and steric effects in aliphatic compounds

SECTION B

NUCLEOPHILIC SUBSTITUTION AT SATURATED CARBON: Mechanism and Stereochemistry of $S_N1$and S_N2, S_Ni reactions. The reactivity effects of substrate structure, solvent effects, competition between $S_N1$and S_N2 mechanisms

SECTION C

ELECTROPHILIC AROMATIC SUBSTITUTION: The Arenium ion mechanism, orientation and reactivity in monosubstituted benzene rings, ortho/ para ratio. Ipso substitution

NUCLEOPHILIC AROMATIC SUBSTITUTION: The Aromatic S_N1, S_N2 and benzyne mechanisms. Reactivtiy – effect of substrate structure, leaving group, and attacking nucleophilic

SECTION D

NEIGHBOURING GROUP PARTICIPATION: Evidences of N.G.P.; the phenonium ion, participation by π and σ bonds, Anchimeric assistance, Classical versus non-classical carbonium ions–the present status

Books recommended

1. M. B. Smith and J. March; March's Advanced Organic Chemistry, 5th Edition, John Wiley & Sons, New York, 2001
2. P. Sykes; A Guide book to Mechanism in Organic Chemistry, 6th Edition, Orient Longman Ltd., New Delhi, 1997
3. S. M. Mukherjee and S.P. Singh; Reaction Mechanism in Organic Chemistry, 1st ed. Macmillan India Ltd., New Delhi, 1990
4. I. L. Finar; Organic Chemistry, Vol. II, 5th Edition, ELBS and Longman Ltd, New Delhi, 1996
5. R.T. Morrison and R.N. Boyd; Prentice: Organic Chemistry, 6thEdition, 1992

Course Title/Code	**Physical Chemistry-I (CHH-503)**
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge of electrochemistry and kinetics of chemical reactions. To impart knowledge of surface chemistry and catalysis
Outcome	Students will be able to understand concepts of electrochemistry and kinetics of chemical reactions Students will be able to understand the role of catalyst on its absorption behavior
Prerequisites	B.Sc. with Chemistry as one of the Subject

SECTION-A

ELECTROCHEMISTRY: Metal/Electrolyte interface: OHP and IHP, potential profile across double layer region, potential difference across electrified interface; Structure of the double layer: Helmholtz-Perrin, Gouy-Chapman, and Stern models. Butler-Volmer equation under near equilibrium and non-equilibrium conditions, exchange current density, Tafel plot. Polarizable and non-polarizable interfaces, Derivation of the Debye-Huckel theory of activity coefficients (both point ion size and finite ion size models

SECTION-B

CHEMICAL KINETICS : Composite Reactions - types of composite mechanisms, rate equations for composite mechanisms, simultaneous and consecutive reactions, steady state treatment, rate determining steps, microscopic reversibility and detailed balance, dynamic chain (H2-Br2) reaction, decomposition of ethane and acetaldehyde) and oscillatory reactions (Belousov-Zhabotinskii reaction), branching chain : H_2-O_2reaction. Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).

SECTION-C

SURFACE CHEMISTRY AND CATALYSIS: Interphase region, curved surfaces. Thermodynamics of surfaces: Gibbs adsorption isotherm, heat and entropy of adsorption. Surface film on liquids;

Electro-kinetic phenomena, Catalytic activity at surfaces (volcano curve), Surface area determination (BET equation), transition state theory of surface reactions: rates of chemisorptions and desorption, unimolecular and bimolecular surface reactions, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity and lateral interaction.

SECTION-D

THERMODYNAMICS: Partial molar properties and their significance. Fugacity: its concept and determination. Properties of ideal solutions; non-ideal systems-deviations (negative and positive) from ideal behaviour, excess functions for non-ideal solutions, calculations of partial molar quantities, determination of partial molar volume and partial molar enthalpy.

Books Recommended

1. O. M. Bockris and A. K. N. Reddy; Modern Electrochemistry, Vol II A & B, 2nd ed. Plenum Press, New York, 1998
2. K. J. Laidler, Harper and Row; Chemical Kinetics, 3rd ed. New York, 1987
3. P. W. Atkins; Physical Chemistry, 7th ed. Oxford University Press, New York, 2002
4. I.N. Levine; Physical Chemistry, 5th ed. Tata McGraw Hill Pub. Co. Ltd., New Delhi, 2002
5. J. Raja Ram and J.C. Kuriacose; Kinetics and Mechanism of Chemical Transformations, MacMillan Indian Ltd., New Delhi, 1992

Course Title/Code	**ANALYTICAL CHEMISTRY (CHH504)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 4-0-0-0
Objectives	To impart knowledge on various analytical techniques To familiarize with the principle of analytical chemometrics
Outcome	Students will be able to Understand various analytical techniques Students will be able to understand factor analysis, resolution and pattern recognition
Prerequisites	B.Sc. with Chemistry as one of the Subject

SECTION A

INTRODUCTION: Scope & objectives, Analytical chemistry and chemical analysis, Classification of analytical methods, Method selection, Sample processing, Steps in a quantitative analysis, Quantitative range (bispartite classification), Data organization, analytical validations, Limit of detection and limit of quantization, The tools of analytical chemistry and good lab practices.

SECTION B

TECHNIQUES IN ANALYTICAL CHEMISTRY-I

Polarography: Origin of polarography, Current-voltage relationship, Theory of polarographic waves (DC and sampled DC (tast) polarograms), Instrumentation, Ilkovic equation, Qualitative and quantitative applications.

SECTION C

TECHNIQUES IN ANALYTICAL CHEMISTRY-II

Spectroscopic Techniques: Theory, Instrumentation and applications of X-rays (emission, absorption, diffraction and fluorescence methods), Atomic absorption Spectroscopy, Atomic fluorescence spectrometry, Atomic emission spectrometry

Spectroscopy: UV-visible molecular absorption spectrometry (instrumentation and application), Molecular luminescence spectroscopy (fluorescence, phosphorescence, chemiluminescence).

SECTION D

TECHNIQUES IN ANALYTICAL CHEMISTRY-III

Separation Methods*:* Principle of chromatography, Classifications of chromatography, Techniques of planar and column chromatography, Gas chromatography, High-performance liquid chromatography

Thermal Analysis: Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC), Principles, techniques and applications of thermometric titration methods

Books Recommended

1. D. A. Skoog; Principles of Instrumental Analysis, 5th ed. Saunders College Publishing, Philadelphia, London, 1998
2. G. W. Ewing; Instrumental Methods of Chemical Analysis, 5th ed. McGraw Hill Books Co, New York, 1978
3. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William; Modern Methods of Chemical Analysis, 2nd ed. John Wiley, New York, 1976
4. J. H. Kennedy, Analytical Chemistry: Principles, 2nd ed. Saunders Holt, London, 1990
5. G. D. Christian; Analytical Chemistry, 5th ed. John Wiley & Sons, New York, 1994
6. D. A. Skoog, D.M. West, F.J. Holler, S. R. Crouch; Analytical Chemistry - An Introduction, 7th ed. Saunders College Publishing, Philadelphia, London, 2000

Course Title/Code	**LABORATORY WORK-I (CHH505)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-8-0
Objectives	To Familiarize students with gravimetric and volumetric analysis of inorganic compounds To Familiarize students with identification of organic compounds having one or more functional groups
Outcome	The students will be able to do gravimetric and volumetric analysis of inorganic compounds The students will be able to understand qualitative analysis of mixture containing five cation
Prerequisites	B.Sc. with Chemistry as one of the Subject

LIST OF EXPERIMENTS

1. To prepare crystals of tetra-amine copper (II) sulphate $[Cu(NH_3)_4]\ SO_4$.
2. To prepare Nickel Dimethylglyoxime Complex $[Ni\ (DMG)_2]$ using Dimethylglyoxime
3. To prepare crystals of Sodium Ferrioxalate $Na_3[Fe(C_2O_4)_3].9H_2O$
4. To estimate magnesium in standard MgSO4 solution using M/100 EDTA in complexometric titration using Eriochrome Black T indicator titrimetrically
5. To estimate amount of calcium in standard CaCO3 solution using M/10 EDTA in complexometric titration using Eriochrome Black T indicator titrimetrically
6. To prepare crystals of Chrome Alum $[K_2SO_4Cr_2(SO_4)_3.24H_2O]$
7. To estimate Aluminium or aluminium oxide in potash alum or ammonium aluminium sulphate.
8. To estimate Ni2+ gravimetrically as Nickel dimethyl glyoxime (Ni-DMG) complex using DMG
9. To estimate Ba2+ gravimetrically as barium chloride

Books Recommended

1. A. Gaddamwar and P. R. Rajput, Organic and Inorganic Practical Chemistry, Pragati Prakashan, 2010
2. R. W. Helmkamp; A Text-book of Practical Organic Chemistry Including Qualitative Organic Analysis, Longman Green and Co. New York, 1956
3. J. Singh and L. D. S. Yadav; Advanced Practical Chemistry, Pragati Prakashan, 2012

Course Title/Code	**Workshop (CHW506)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-3-0
Objectives	To Familiarize students with inorganic synthesis To expose the students with the synthesis of organic compounds and intermediates. To familiarize students with conductometric and potentiometric titrations.

INORGANIC ANALYSIS:

1. Qualitative analysis of mixtures of salts including rare element salts (soluble and insoluble) containing eight radicals including interfering
2. Qualitative analysis of mixtures of metal ions by complexometric titrations (mixture of two metals) with the use of masking and demasking agents.
3. TLC : preparation and analysis
4. Preparation of compounds and intermediates involving up to two steps.
5. Determination of solubility product of sparingly soluble salt conductometrically.
6. Conductometric titration of a mixture of weak and strong acids.

Books Recommended

1. A. Gaddamwar and P. R. Rajput, Organic and Inorganic Practical Chemistry, Pragati Prakashan, 2010

2. R. W. Helmkamp; A Text-book of Practical Organic Chemistry Including Qualitative Organic Analysis, Longman Green and Co. New York, 1956
3. J. Singh and L. D. S. Yadav; Advanced Practical Chemistry, Pragati Prakashan, 2012

Course Title/ Code	**Research Methodology/PHS 501**
Course Type	**Allied Core**
Course Nature	**Soft**
L-T-P Structure	**(1-0-2)**
Objectives	Student shall be able to apply the fundamentals of research methodology to a problem and make an informed decision.
Outcome	Student shall be able to 1. Write hypothesis; generate and choose alternatives; and test hypothesis. 2. Select a sample ; generate data and present it 3. Calculate averages and dispersion 4. Calculate correlation and regression.

SECTION A

Basic Concepts of Research; Formulation & steps of Research: Decision-making: identifying the problem & Steps of decision-making process. Research: Its objectives and types, Formulation of Research Problem; its components and sources, steps of research & research ethics, performance monitoring in research

Research Design: Requirements of Research Design; Types of Research Design; Factors Affecting Research Design; Hypothesis Formulation; Hypothesis Testing

SECTION B

Sampling Methods and Techniques: Sampling design; Scope of sampling method; Laws of sampling; Determination of sample size; Techniques of sampling**.**

Properties of Data Collection and Measurement: Basic Characteristics of data; Types of data and Scaling measurement. Methods of primary data collection; Editing Raw Data; Coding of Data; Tabulation of Data; Constructing Charts.

Presentation of Results: Report writing: Purpose of a Report; Essentials of a Good Report; Format of a Report; Types of Report Presentation.

SECTION C

Measures of Central Tendency: Types of Averages: The Arithmetic Mean; The Weighted Arithmetic Mean; The Median; The Mode; The Geometric Mean; The Harmonic Mean

Measures of Dispersion: Definition; Methods of Measuring Dispersion; The Range; The Inter-quartile Range; The Mean/Average Deviation ; The Standard Deviation; The Coefficient of Variation; The Gini Coefficient and the Lorenz Curve

Matrix Algebra : Matrix Multiplication; Matrix Addition; Matrix Substitution; Transpose of the Product of Two Matrices; Inverse of a Square Matrix; Matrix Notation in Case of Regression Analysis

SECTION D

Multivariate Analysis; Correlation & Regression Analysis: Factor Analysis; Discriminant Analysis; Cluster Analysis; Dimensional Analysis; Meta Analysis; Conjoint Analysis. Introduction to Correlation Analysis; Rank Correlation; Linear Regression Analysis; Multiple Regression Analysis

List of Experiments:

1. Identifying the hypothesis; alternatives and situations in given abstracts/reports.
2. Writing a research proposal as per research design fundamentals.
3. Coding, tabulating and drawing charts for a given data.
4. Calculating & plotting averages for the given data
5. Measuring dispersion for the given data.
6. Calculating correlation for the given data.
7. Calculating regression for a given data.

Mini Project: Identify a problem in given environment and apply the concepts of research methodology to conduct research and present the results.

Books Recommended:

1. P. Sarangi; Research Methodology, Taxmann Publications Pvt Ltd., 2010
2. C. R. Kothari; Research Methodology methods and Technique, 3rd ed. New Age International Pvt Ltd., 2004

SEMESTER II

DETAILED SYLLABUS
SEMESTER II

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core(Departmental/ Allied)/ Elective (Departmental/ Open) / University Compulsory	Hard/Soft/ Workshop/ NTCC						
CHH508-T	INORGANIC CHEMISTRY-II	CORE(Departmental)	HARD	4	0	0	0	4	4
CHH509-T	ORGANIC CHEMISTRY-II	CORE(Departmental)	HARD	4	0	0	0	4	4
CHH510-T	PHYSICAL CHEMISTRY-II	CORE(Departmental)	HARD	4	0	0	0	4	4
CHH511-T	SPECTROSCOPY	CORE(Departmental)	HARD	4	0	0	0	4	4
CHH512-P	LABORATORY WORK-II	CORE(Departmental)	HARD	0	0	8	0	8	4
CHW513	WORKSHOP	CORE(Departmental)	WORKSHOP	0	0	3	0	3	2
MES 515	RESEARCH PAPER WRITING	CORE (Allied)	SOFT	1	0	2	0	3	2
CHW514	SUMMER TRAINING								3

Course Title/Code	Inorganic Chemistry-II (CHH508)
Course Type	Core
Course Nature L-T-P-O Structure	Hard 4-0-0-0
Objectives	To familiarize with kinetics of substitution reactions To impart knowledge on electron transfer reactions
Outcome	The students will be able to understand Kinetics and Mechanism of Substitution Reactions The students will be able to understand electron transfer reaction
Prerequisites	Inorganic Chemistry-I

SECTION-A

KINETICS AND MECHANISM OF SUBSTITUTION REACTIONS: Nature of substitution reactions; prediction of reactivity of octahedral, tetrahedral, trigonal bipyramidal and square-planar complexes in terms of VBT and CFT; rates of reactions; acid hydrolysis, base hydrolysis and anation reactions.

SECTION-B

ELECTRON TRANSFER REACTIONS: Mechanism and rate laws; various types of electron transfer reactions, Marcus-Husch theory, correlation between thermal and optical electron transfer reactions; identification of inter valence transfer bands in solution.

SECTION-C

METAL CARBONYLS: Preparation and structure; vibrational spectra of metal carbonyls, reactions of metal carbonyls.

SECTION-D

OPTICAL ROTATORY DISPERSION AND CIRCULAR DICHROISM: Linearly and circularly polarized lights; optical rotatory power and circular birefringence, elipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects; Assignment of electronic transitions; applications of ORD and CD for the determination of (i) absolute configuration of complexes and (ii) isomerism due to non-planarity of chelate rings.

Books Recommended

1. F. Basalo and R. G. Pearson; Mechanism of Inorganic Reactions, 2nd ed. Wiley Eastern Ltd., New Delhi, 1967
2. D. F. Shriver and P. W. Atkins; Inorganic Chemistry, 3rd ed. ELBS, London, 1999
3. F. A. Cotton and G. Wilkinson; Advanced Inorganic Chemistry, 6th ed. John Wiley & Sons, New York, 1999
4. D. N. Sathyanarayana; Electronic Absorption Spectroscopy and Related Technique, Universities Press (India) Ltd., Hyderabad, 2001
5. K. F. Purcell, J. C. Kotz; Inorganic chemistry, Saunders, 1977

Course Title/Code	Organic Chemistry-II (CHH509)
Course Type	Core
Course Nature L-T-P-O Structure	Hard 4-0-0-0
Objectives	To familiarize with electrophilic, free-radical and nucleophilic addition reactions To impart knowledge on esterification and Elimination reactions
Outcome	Students will be able to understand the mechanism of electrophilic, free-radical and nucleophilic addition reactions Students will be able to explain the mechanism of esterification and Elimination reactions
Prerequisites	Organic Chemistry-I

SECTION A

ADDITION TO CARBON–CARBON MULTIPLE BONDS: Electrophilic, free-radical and nucleophilic addition: Mechanistic and Stereo chemical aspects. Orientation and reactivity, Hydroboration and Michael reaction

SECTION B

ESTERIFICATION AND HYDROLYSIS OF ESTERS: Evidence for tetrahedral intermediate in BAc2 and AAc2 mechanisms, steric and electronic effects. The AAc1 and other pathways involving alkyl to oxygen bond cleavage

SECTION C

ELIMINATION REACTIONS: The E1, E2 and E1Cb (Elimination Unimolecular conjugate Base) mechanisms, Orientation of the double bond. Hofmann versus Saytzeff elimination, Pyrolytic syn-elimination, Competition between substitution and elimination reactions

KINETIC ISOTOPE EFFECTS: Its origin and importance in determining reaction mechanism, Solvent isotope effects.

SECTION D

CONSERVATION OF ORBITAL SYMMETRY IN PERICYCLIC REACTIONS: Woodward-Hoffmann rules; cycloaddition [2+2] and [4+2], and electrocylic reactions, Prototropic and Sigmatropic rearrangements, Ene reactions and Cheletropic reactions; 1,3-Dipolar cycloaddition

Books recommended

1. M. B. Smith and Jerry March; March's Advanced Organic Chemistry, 5th ed. John Wiley & Sons, New York, 2001
2. P. Sykes; A Guide Book to Mechanism in Organic Chemistry, 6th ed. Orient Longman Ltd., New Delhi, 1997
3. S. M. Mukherjee and S.P. Singh; Reaction Mechanism in Organic Chemistry, 1st ed. Macmillan India Ltd., New Delhi, 1990

4. T. H. Lowry and K. S. Richardson; Mechanism and Theory in Organic Chemistry, 3rd ed. Addison – Wesley Longman Inc., 1998
5. P. S. Kalsi; Organic Reactions and Their Mechanisms, 1st ed. New Age International Pub., New Delhi, 1996

Course Title/Code	Physical Chemistry-II (CHH510)
Course Type	Core
Course Nature L-T-P-O Structure	Hard 4-0-0-0
Objectives	To familiarize with concept of corrosion cyclic voltammetry To impart knowledge of Statistical Thermodynamics
Outcome	Students will be able to understand corrosion cause and type Students will be able to understand Statistical Thermodynamics in relation to the Concepts of distribution and thermodynamic probability
Prerequisites	Physical Chemistry-I

SECTION-A

ELECTROCHEMISTRY: CORROSION: Scope and economics of corrosion, causes and types of corrosion, electrochemical theories of corrosion, kinetics of corrosion (corrosion current and corrosion potential), Corrosion measurements (weight loss, OCP measurement, and polarization methods), units of corrosion rate passivity and its breakdown, corrosion, prevention (electrochemical, inhibitor, and coating methods)

CYCLIC VOLTAMMETRY: Cell design, instrumentation, current-potential relation for linear sweep voltammetry (LSV), cyclic voltammetry.

SECTION-B

STATISTICAL THERMODYNAMICS: Concepts of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Boltzmann distribution of particles. Types of statistics: Maxwell- Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Idea of microstates and macrostates, Thermodynamic probability (W) and derivation of distribution laws for three types of statistics

PARTITION FUNCTION: translational, rotational, vibrational partition functions, thermodynamic properties of ideal gases in terms of partition function.

SECTION-C

MICELLES: Surface active agents and their classification, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsions, reverse micelles.

MACROMOLECULES: Polymers-definition, types of polymers, liquid crystal polymers. Molecular mass-number and mass average molecular mass, determination of molecular mass (osmometry, viscosity, diffusion, light scattering, and sedimentation methods).

SECTION-D

NUCLEAR CHEMISTRY: Nuclear stability and binding energy, Mass and binding energy systematic, Nuclear isomerism and internal conversion, Nuclear fission and nuclear fusion- fission cross section, chain fission, fission product and fission yield, mass and charge distribution in fission, Nuclear fusion and stellar energy.

Books Recommended-

1. J. O. M. Bockris and A. K. N. Reddy; Modern Electrochemistry, Vol II, 2nd ed. Plenum Press, New York, 1998
2. P. W. Atkins; Physical Chemistry, 7th ed. Oxford University Press, New York, 2002
3. I. N. Levine; Physical Chemistry, 5th ed. Tata McGraw Hill Pub. Co. Ltd., New Delhi, 2002
4. A. Maczek; Statistical Thermodynamics, Oxford University Press Inc., New York, 1998
5. Y. Moroi; Micelles: Theoretical and Applied Aspects, Plenum Press, New York, 1992
6. F. W. Billmayer; Text Book of Polymer Science, 3rd ed. Wiley-Interscience, New York, 1984
7. B. G. Harvey; Introduction to Nuclear Physics and Chemistry, Prentice Hall, Inc, 1969
8. H. J. Arnikar; Essentials of Nuclear Chemistry, 4th ed. Wiely-Estern Ltd., New Delhi, 1995

Course Title/Code	**SPECTROSCOPY (CHH511)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 4-0-0-0
Objectives	To familiarize with PMR and CMR To impart knowledge on mass spectroscopy for studying the fragmentation pattern
Outcome	Students will be able to understand principle of PMR, CMR and ESR spectroscopy Students will be able to understand Photoelectron Spectroscopy Students will be able to analysis fragmentation pattern of the compound by mass spectrometry
Prerequisites	B.Sc. with Chemistry as one of the Subject

SECTION A

SPECTROSCOPY-I

PMR: Natural abundance of ^{13}C, ^{19}F and ^{31}P nuclei, the spinning nucleus, effect of external magnetic field, precessional motion and frequency Energy transitions Chemical shift and its measurements, factors influencing chemical shift, anisotropic effect, integral of protons spin spin coupling splitting theory magnitude of coupling constant simple, virtual and complex spin coupling , Chemical and magnetic equivalence proton exchange, factors affecting the coupling- First and non first order spectra, simplification of complex spectra (solvent effect, double resonance and field effect)

SECTION B

CMR: Resolution and multiplicity of ^{13}C NMR, ^{1}H-decoupling noise decoupling, broad band decoupling, Deuterium, fluorine and phosphorus coupling, NOE signal enhancement off-resonance, proton decoupling, structural application of CMR DEPT and INEPT experiments, Introduction to 2D NMR .

SECTION C

ESR: Derivative curves hyperfine splitting, g value, ESR spectra of simple molecules

Mass: Theory, instrumentation and modification Unit mass and molecular ions Important terms singlv, double/multiple charged ion metastable peak base peak isotopic mass peak, relative intensity etc.

SECTION D

Photoelectron Spectroscopy: Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N2, O2, F2, , CO, HF, NH3 and H2O - Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M+) species, Prediction of Nature of Molecular Orbitals. ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Books Recommended-

1. R. M. Silverstein, D. J. Kiemle and F. X. Webster; Spectroscopic identification of organic compounds, 7th ed. John Wiley & sons, 2005

2. William Kemp; Organic spectroscopy 3rd ed. Palgrave publishing house, 2008

3. M. Rose and R. A. W. Johnstone; Mass Spectrometry for Chemists and biochemists, 2nd ed. Cambridge University Press, 2012

4. D. H. Williams and I. Fleming; Spectroscopic methods in organic chemistry, 6th ed. McGraw Hill Publishing Co. 1989

Course Title/Code	**LABORATORY WORK-II (CHH512)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-8-0
Objectives	To familiarize students with Quantitative separation and determination of metal ions
Outcome	Students will be able to understand Quantitative separation and determination of metal ions
Prerequisites	Nil

INORGANIC CHEMISTRY PRACTICALS

1. Quantitative separation and determination of the following pairs of metal ions using gravimetric and volumetric methods. For example: Ag^{+} (gravimetrically) and Cu^{2+} (volumetrically), Cu^{2+} (gravimetrically) and Zn^{2+} (volumetrically), Fe^{3+} (gravimetrically) and Ca^{2+} (volumetrically), Mg^{2+} (gravimetrically) and Ca^{2+} (volumetrically) etc.

ORGANIC CHEMISTRY PRACTICALS

1. Preparation of compounds involving not more than two steps.
2. Identification of organic compounds in given mixture.

PHYSICAL CHEMISTRY PRACTICALS

1. Rate constant of acid catalyzed hydrolysis of sucrose by polarimetric method.
2. Rate constant of acid catalyzed hydrolysis of sucrose by chemical method.
3. Rate constant of $FeCl_3$-catalyzed H_2O decomposition by gasometric method.
4. Degree of hydrolysis of urea hydrochloride by kinetics method.

Books recommended:

1. A. Gaddamwar and P. R. Rajput; Organic and Inorganic Practical Chemistry, Pragati Prakashan, 2010
2. R. W. Helmkamp; A Text-book of Practical Organic Chemistry Including Qualitative Organic Analysis, Longman Green and Co. New York, 1956
3. J. Singh and L. D. S. Yadav; Advanced Practical Chemistry, Pragati Prakashan, 2012

Course Title/Code	**Workshop (CHW513)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-3-0
Objectives	To familiarize students with Preparation of compounds involving not more than two steps To expose the students with polarimetric method to determine rate constant.

LIST OF EXPERIMENTS

1. Separation of a mixture of cations/anions by paper chromatographic technique using aqueous/non- aqueous media. For example: Pb2+ and Ag+ (aqueous & non-aqueous media),$Co^{2+}$and Cu^{2+} (non-aqueous medium), Cl^- and I^- (aqueous-acetone medium),Br^- and I^- (aqueous-acetone medium) etc.
2. Systematic identification of mixtures containing two organic compounds
3. Equilibrium constant of $KI + I_2 \Leftrightarrow KI_3$ by distribution method.

Books Recommended

1. A. Gaddamwar and P. R. Rajput; Organic and Inorganic Practical Chemistry, Pragati Prakashan, 2010
2. R. W. Helmkamp; A Text-book of Practical Organic Chemistry Including Qualitative Organic Analysis, Longman Green and Co. New York, 1956
3. J. Singh and L. D. S. Yadav; Advanced Practical Chemistry, Pragati Prakashan, 2012

Course Title/ Code	RESEARCH PAPER WRITING
Course Code	MES 515
Course Type	DOMAIN CORE
Course Nature	SOFT COURSE
L-T-P-O Structure	1-0-2-0
Objectives	To acquaint the researcher with the tools of research by exposing them to the mechanics of writing a research report/ research paper/ thesis/ dissertation.
Learning Outcomes	Upon completion of this course, the students should be able to: • Know what formats, designs, structure and styles to use to best get their ideas, concepts and messages across in a way that is clear and unambiguous. • Be capable of recognizing and correcting many common errors that currently occur within written communication in the technical field. • Use clear and powerful language to target and persuade readers for positive results

SECTION A

Research Paper:- Definition, Quality of a good Research Paper, Report Paper and Thesis Paper; Details of a Research Paper – Steps and Schedule. **Choosing a Topic**: Brainstorming, Consulting Experts, Considering Parameters, Narrowing the Research Topic, **Thesis**: Definition and function, Outline, Thesis Statement

SECTION B

Doing Research:- Finding Information, Sources of Information; Online Resources, Search Engines, Databases, Newsgroups, Internet Sites; Library – Books, Research Papers, Periodicals, Magazines and Journals,, Interviews, Surveys, Government Documents, Pamphlets, Special Collections; Evaluating Sources, **Taking Notes**:- Reading, Notes Taking Methods, Guidelines and Summarizing

SECTION C

Rough Draft :- Transforming Notes into Rough Draft Creating Outlines, Types of Outlines; Basics of Research Paper Style ; Words, Sentences, Punctuation ; Writing Introduction; Using Notes, Quotations, Graphics, etc, **Revising Rough Drafts**: Principles, Revising Opening Paragraph, Sentences, Words and Rules for Writers, Plagiarism and how to avoid it, Plagiarism Detection Programs

SECTION D

Documentation: MLA System of Documentation; Parenthetical Documentation, Format for Work Cited, Using Footnotes and Endnotes to Document Sources and add Observations and Comments – Guidelines and Format; APA System of Documentation, Traditional System of Documentation (CMS).
Presentation of Research Paper: Title Page, Table of Contents, Forward and Preface, Abstract, Presentation Footnote. Finished Form of Paper – Revising, Editing, Proofreading, Peer Review Checklist, Submitting Electronically, Model Research Papers

Reference Books:

1) J. Gibaldi; MLA Handbook for Writers of Research Papers, 7th ed. New Delhi: East-West Press, 2009
2) C. R. Kothari; Research Methodology: Methods and Techniques, 2nd ed. New Age International Ltd, New Delhi, 1985.
3) F. A. Rahim; Thesis Writing: A Manual for Researchers, New Age International Pvt Ltd, New Delhi, 1996.
4) R. Laurie; Schaum's Quick Guide to Writing Great Research Papers, McGraw- Hill Publishing House, New York, 2007.
5) C. W. Anthony and M. M. Jo Ray; Writing the Research Paper, Wadsworth Cengage Learning, 2008

LABORATORY

Report writing consisting of about 1,000 words, on any subject of the student's choice, in the field of research in Mechanical Engineering

Prepare atleast two Research Papers in IEEE & Science Direct Format. Your **research paper** must be 3 pages **minimum** plus reference page, typed (approx. 250 words per page) on a technical topic of the student's choice dealing the field of research in Mechanical.

Seminar presentation, on Report Writing and Research Papers

SEMESTER III

(Organic Specialization)

Organic Specialization
SEMSETER III

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core (Departmental/ Allied)/ Elective Departmental/ Open)/ University compulsory	Hard/ Soft/ Workshop / NTCC	L	T	P	O		
CHH615	CONFORMATIONAL ANALYSIS, ASYMMETRIC SYNTHESIS & BIOMOLECULES	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH616	MODERN ORGANIC SYNTHETIC TECHNIQUES & STEREOCHEMISTRY	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH617 CHH618	ELECTIVE-I (A) BIO-INORGANIC CHEMISTRY AND ORGANOMETALLIC CHEMISTRY & (B) DRUG DESIGN	ELECTIVE (Departmental)	HARD	4	0	0	0	4	4
CHH619	PHOTOCHEMISTRY & PERICYLIC REACTIONS	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH620	LABORATORY WORK-III	CORE (Departmental)	HARD	0	0	6	0	6	3
CHH621	LABORATORY WORK-IV	CORE (Departmental)	HARD	0	0	6	0	6	3
CHN622	SEMINAR	CORE (Departmental)		0	0	0	2	2	2

DETAILED SYLLABUS
SEMESTER III

Course title/code	CONFORMATIONAL ANALYSIS AND ASYMMETRIC SYNTHESIS & BIOMOLECULES (CHH615)
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To make the students familiarize about the conformations of basic organic compounds To introduce to the students the basic terminology, nomenclature and conditions involved in asymmetric synthesis To familiarize the students with the enzyme catalyzed reactions To make the students understand the structures of various nucleic acids
Outcome	The student will be able to learn about the conformational analysis of various organic compounds The student will be able to understand the principles of asymmetric syntheses The student will be able to write the mechanism of enzyme catalyzed reactions and synthesis of nucleic acids
Prerequisites	Organic Chemistry-I & II

SECTION A

CONFORMATIONAL ANALYSIS (CYCLIC SYSTEMS): Study of conformations of cyclohexane, mono, di and polysubstituted cyclohexanes, cyclohexene, cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cyclopentane, cyclobutane, cycloheptane and cyclooctane, Stereochemistry of bicycle [3,3,0]octanes, hydrindanes, decalins and perhydroanthracenes.. Conformaitonal effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereo electronic factors – examples, Factors governing the reactivity of axial and equatorial substituents in cyclohexanes, Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

SECTION B

PRINCIPLES OF ASYMMETRIC SYNTHESIS: Introduction and terminology: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Stereoselective reactions: Substrate stereoselectivity, product stereoselectivity, enantioselectivity and diastereoselectivity. Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity. Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio.

SECTION C

METHODOLOGIES IN ASYMMETRIC SYNTHESIS: Strategies in Asymmetric Synthesis: l. Chiral substrate controlled, 2. Chiral auxiliary controlled, 3. Chiral reagent controlled and 4. Chiral catalyst controlled.

1. Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

2. Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, azaenolates, imines and hydrazones. 1, 4 Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder reaction.
3. Asymmetric aldol reaction: Diastereoselective aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

SECTION D

1. ENZYMES: Definition, Classification based on mode of action, Mechanism of enzyme catalysis, Lock and Key model and Induced- Fit model, Enantiomer, discrimination by Three- point Contact model. Factors affecting enzyme catalysis. Enzyme inhibition- reversible and irreversible inhibition, Enzymes in organic synthesis. Immobilised enzyme

2. NUCLEIC ACIDS: Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA, Replication, transcription and translation, Genetic code, Protein biosynthesis, Chemical Synthesis of nucleosides and nucleotides

Books Recommended

1. D. Nasipuri; Stereochemistry of Organic Compounds-Principles & Applications, 4th ed. New Age International Pvt Ltd, 2012
2. P. S. Kalsi; Stereochemistry of Organic Compounds- Conformation and Mechanism, 8th ed. New Age International Pvt Ltd, 2015
3. R.T. Morrison and R.N. Boyd; Organic Chemistry, 6th ed. Prentice Publishing, 1992
4. E. L. Eliel and S. H. Wilen; Stereochemistry of Organic compounds, Wiley Chichester, 1994
5. R. S. Ward; Stereo selectivity in organic synthesis, 1st ed. Wiley Chichester, 1999
6. M. Nogradi; Stereoselective Synthesis. 1st ed. VCH Publisher, USA, 1987

Course title/code	**MODERN ORGANIC SYNTHETIC TECHNIQUES & STEREOCHEMISTRY (CHH616)**
Course Type	Core
Course Nature	Elective
L-T-P-O Structure	4-0-0-0
Objectives	To familiarize the student with the various synthetic reagents for using group protection and oxidation reactions. To make the student understand the mechanism of various synthetic routes. To make the student understand the new techniques and concepts in organic synthesis Student will be familiarized with stereochemistry principles.
Outcome	The student will be able to write the mechanism of organic reactions. The student will be able to predict the structure of organic compounds by stereochemistry.
Prerequisites	Organic and Inorganic Chemistry-I & II

SECTION A

REAGENTS IN ORGANIC SYNTHESIS AND NAME REACTIONS

Named Reactions: Cannizzaro reaction, Hell-VolhardZelinssky reaction, Oppenauer oxidation, Parkin reaction and Birch reduction. Reagents- Aluminiumisopropoxide, N-Bromosuccinimide, Lithium aluminium hydride, boron trifluoride, Raney NI, Sodium borohydride, Periodic acid, Osmium tetraoxide, Fentons reagent and di-azo methane

SECTION B

MEHTODS OF ORGANIC SYNTHESIS

Oxidation, Reduction and Cyclization approach of synthesis, Acidity of alpha hydrogen atom, Alkylation in organic synthesis, protection of groups, functional group interaction, disconnection approach, solute-solvent effect on productivity, chemo selectivity.

SECTION C

PHASE TRANSER CATALYSIS IN ORGANIC SYNTHESIS

Definition, Mechanism of PTC reactions, trpes of PTC catalyst (Tetra hexyl ammonium bromide, hexadcyltribuylphosphomonium bromide, tetrahexyl ammonium hydrogen sulhate, tetra butyl ammonium hydrogen sulhate, benzyl triethyl ammonium chloride), advantags of PTC reactions, preparation (Quaternary salts and exchange of anions on quaternary salts), application of PTC (nitriles from alkyl halides, benozyl cyanides from benozylchrlodies, alkyl nitrates, thiocynates, cyanides form alkyl halides), Alkylations, Michel reactions, witig reactions etc

SECTION D

Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.

Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.

Asymmetric synthesis:Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination, Resolution – optical and kinetic

Books Recommended

1. M. B. Smith and Jerry March; March's Advanced Organic Chemistry, 5th ed. John Wiley & Sons, New York, 2001
2. F. A. Carey and R. J. Sundberg; Advanced Organic Chemistry, 5th ed. Springer Publishers, 2008
3. R.T. Morrison and R.N. Boyd; Organic Chemistry, 6th ed. Prentice Publishing, 1992
4. H. O. House, W. A. Benjamin; Modern Organic Reactions, 2nd ed. VCH Publishers, USA, 1972
5. R. O. C. Norman and J. M. Coxon; Principles of Organic Synthesis, 3rd ed. Blackie Academic & Pro, 1993
6. S. M. Mukherji and S. P. Singh; Reaction Mechanism in Organic Chemistry, 3rd ed. Macmillan, 1984
7. D. Nasipuri; Stereochemistry of Organic Compounds–Principles & Applications, 3rd ed. New Age International Pvt Ltd, 2014

Course title/code	PHOTOCHEMISTRY AND PERICYLIC REACTION (CHH619)
Course Type	Core
Course Nature L-T-P-O Structure	Hard 4-0-0-0
Objectives	The student will be exposed to photochemistry of various electronic transitions The student will be introduced to various pericylic reactions and their mechanisms
Outcome	The student will be able to write mechanism of various pericylic reactions. Student will understand photochemistry of various electronic transition **(π-π* and n-π*)**
Prerequisites	Organic Chemistry-I & II

SECTION-A

PHOTOCHEMISTRY OF (Π-Π*) TRANSITIONS: Excited states of alkenes, cis-trans isomerisation, photostationary state, electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Intermolecular reactions, photo cycloadditions, photodimerisation of simple and conjugated olefins, addition of olefins to α, β-unsaturated carbonyl compounds, excited states of aromatic compounds, Photoisimerisation of benzene

SECTION-B

PHOTOCHEMISTRY OF (N-Π*) TRANSITIONS: Excited states of carbonyl compounds, homolytic cleavage of α- bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkanediones, Intermolecular abstraction of hydrogen: photoreduction - influence of temperature, solvent, nature of hydrogen donor and structure of the substrate Intramolecular abstraction of hydrogen:Norrish type II reactions in ketones, Esters and 1, 2- diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.

SECTION-C

PERICYCLIC REACTIONS I INTRODUCTION - Characteristics and classification of pericyclic reactions—Electrocyclic, cycloaddition & cycloreversions and sigmatropic reactions—4ne and 4n+2e type examples, Approaches for the interpretation of mechanism of pericyclic reactions-Aromatic Transition States (ATS)/Perturbation, Molecular Orbitals (PMO) approach-Concept of Huckel – Mobius aromatic and antiaromatic transition states, Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach, Solving problems based on ATS approach.

SECTION-D

PERICYCLIC REACTIONS II

Molecular orbitals-definition and their origin-Non-mathematical writing up of molecular orbitals and their symmetry properties for acyclic conjugated systems, Frontier Molecular Orbital (HOMO LUMO) approach-concept-Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach, Solving problems based on FMO approach, Conservation of orbital symmetry (Correlation Diagrams) approach-concept- Framing Woodward-

Hofmann selection rules for electrocylic and cycloadditions & cycloreversions by Conservation of orbital symmetry approach.

Books Recommended

1. J. Singh and J. Singh; Photochemistry and Pericyclic reactions, 3rd ed. New Age International Pvt Ltd, 2005
2. S. Sankararaman; Pericyclic Reactions- A text Book, 1ST ed. Wiley VCH, 2005
3. W. Horsepool; Handbook of Organic Photochemistry and Photobiology, 1st ed. CRC Press, 1984

Course Title/Code	LABORATORY WORK-III (CHH620) Common
Course Type	Core
Course Nature L-T-P-O Structure	Hard 0-0-6-0
Objectives	To familiarize with synthesis of organic compounds
Outcome	The student will be able to understand isolation of natural products
Prerequisites	Organic Chemistry-I & II

LIST OF EXPERIMENTS

SEPARATION & ANALYSIS OF ORGANIC COMPOUNDS

1. Mixture of mannitol and p-toluidine
2. Mixture of glucose and cinnamic acid
3. Mixture of oxalic acid and m-dinitrobenzene or p-dinitrobenzene
4. Mixture of urea and acetanilide
5. Mixture of benzyl and p-toluidine
6. To prepare Hexammine cobalt (II) Chloride
7. To prepare Copper tetra iodide mercurate
8. To prepare Vanadyl acetyloacetonate
9. To prepare Dichlorodipyridinocobalt (II)
10. To prepare ammonium diammine tetrathiocyanato chromate (III)

Books Recommended:

1. J. Singh, R. K. P. Singh, J. Singh, L. D. S. Yadav, I. R. Siddiqui and J. Srivastava; Advanced Practical Chemistry, 2nd ed. Pragati Prakashan, 2010
2. A. I. Vogel; Vogel's textbook of Practical Organic Chemistry, 5th ed. Longman Scientific and technical Publisher, UK, 1989
3. H. L. Fieser and F. L. Fieser, Organic Chemistry, Vol 1-11, Trade ed. 1944

Course Title/Code	LABORATORY WORK-IV (CHH621)
Course Type	Core
Course Nature L-T-P-O Structure	Hard 0-0-6-0

Objectives	To familiarize with Multistage synthesis. To impart knowledge on isolation of natural products.
Outcome	The students will be able to understand enzymatic reaction and application of phase transfer catalysis
Prerequisites	Organic Chemistry-I & II

LIST OF EXPERIMENTS

TO SEPARATE AND ANALYSE THE ORGANIC COMPOUNDS

1. Mixture of benzoic acid and β-naphthol
2. Mixture of m-notroaniline and hydroquinone
3. Mixture of tetrahydrofuran and cinnamic acid
4. Mixture of chloroform and benzidine
5. Mixture of aniline and benzamide
6. To prepare Chalcone (Benzene acetophenone)
7. To extract caffeine from tea leaves
8. To extract piperine from Black pepper

Recommended Books:

1. J. Singh, R. K. P. Singh, J. Singh, L. D. S. Yadav, I. R. Siddiqui and J. Srivastava; Advanced Practical Chemistry, 2nd ed. Pragati Prakashan, 2010
2. A. I. Vogel; Vogel's textbook of Practical Organic Chemistry, 5th ed. Longman Scientific and technical Publisher, UK, 1989
3. H. L. Fieser and F. L. Fieser, Organic Chemistry, Vol 1-11, Trade ed. 1944Vogel Practical Organic Chemistry.
4. B. M. Trost, I. fleming and S. L. Scheiber; Comprehensive Organic Synthesis, 1st ed. Pergamon Press, 2007

Course Title/Code	**Seminar (CHN622)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-0-2
Objectives	To impart understanding of research papers/articles in specific areas To improve the communication skills by presentation on specific subjects

SEMESTER III

(Inorganic Specialization)

Inorganic Specialization
Semester III

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core(Departmental/Allied)/Elective Depart-mental/ Open) / University Compulsory	Hard/Soft/ Workshop/ NTCC	L	T	P	O		
CHH629	Instrumentation techniques and separation methods	CORE(Departmental)	HARD	4	0	0	0	4	4
CHH630	Solid State Chemistry & its Applications	CORE(Departmental)	HARD	4	0	0	0	4	4
CHH617 CHH618 CHH631	ELECTIVE-I A. BIOINORGANIC CHEMISTRY & ORGANOMETALLIC CHEMISTRY B. DRUG DESIGN C. POLYMER CHEMISTRY	CORE(Departmental)	ELECTIVE	4	0	0	0	4	4
CHH632	Metal Clusters and Advanced Coordination Chemistry	CORE(Departmental)	HARD	4	0	0	0	4	4
CHH620	LABORATORY WORK-III	CORE(Departmental)	HARD	0	0	6	0	6	3
CHH633	LABORATORY WORK-IV	CORE(Departmental)	HARD	0	0	6	0	6	3
CHN622	SEMINAR	CORE(Departmental)		0	0	0	2	2	2

DETAILED SYLLABUS

CHP01 – THIRD SEMESTER

Course Title/Code	**Instrumentation Techniques and Separation Methods (CHH629)**
Course Type	**Core**
Course Nature	**Hard**
L-T-P-O Structure	**4-0-0-0**
Objectives	**To familiarize students with the principles, working and applications of various instruments**
Outcome	**Students will be able to recognize the use of various instruments to different fields of Inorganic Chemistry**
Prerequisites	**A knowledge of Inorganic ions and basics behind the spectra generations**

SECTION-A

Optical methods – Electronic spin resonance spectra, Atomic absorption spectroscopy, Mossbauer spectroscopy, IR spectroscopy (Far IR and near IR), Raman Spectroscopy, Difference between Raman and IR spectra, Emission spectra

SECTION B

Separation methods – Theory and applications of separations methods: solvent extraction, rotavapor distillation;

Spectral analysis of the Chromatographic Techniques

HPTLC: its instrumentation, working, applications to inorganic species and limitations,

HPLC: Type of stationary (reverse phase, normal phase, ion exchange, hydrophobic and hydrophilic interaction, chiral) Mobile phase (isocritical gradient), detecters (UV, RI and PDA), working, applications to inorganic species and limitations,

Supercritical Chromatography, Capillary electrophoresis, Potentiometry, Coulometry, Voltametry

SECTION C

Imaging Techniques – SEM, TEM and HRTEM; **Diffraction methods** – single crystal and powder XRD & their applications for inorganic compounds, neutron diffraction & electron diffraction, Introduction and Principle of AFM and XPS

SECTION D

Spectroscopic and hyphenated techniques: BET, FT–IR, GC-IR, GC-MS, LC-MS, TLC-MS, ICP-MS working instrumentation, applications and limitations

Recommended Books

1. D.A. Skoog; Principles of Instrumental Analysis, 5th ed. Saunders College Publishing, Philadelphia, London, 1998
2. G.W. Ewing; Instrumental Methods of Chemical Analysis, 5th ed. McGraw Hill Books Co., New York, 1978

3. J.H. Kennedy; Analytical Chemistry: Principles, 2nd ed. Saunders Holt, London, 1990
4. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William; Modern Methods of Chemical Analysis, 2nd ed. John Wiley, New York, 1976
5. G. D. Christian; Analytical Chemistry, 5th ed. John Wiley & Sons, New York, 1994.
6. D. A. Skoog, D.M. West, F.J. Holler and S.R. Crouch; Analytical Chemistry - An Introduction, 7th ed. Saunders College Publishing, Philadelphia, London, 2000

Course Title/Code	Solid state chemistry and its applications (CHH 630)
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To familiarize students with the concept of solid crystals, defects and their packaging system
Outcome	Students will be able to understand the compositional and structural aspects of inorganic solid substance
Prerequisites	Inorganic Chemistry I and II

SECTION-A

Crystal structure of inorganic compounds: close packing, packing efficiency, interstitial sites, limiting radius ratios, ionic crystals containing two or three different elements – NaCl, ZnS, CsCl, CaF_2, TiO_2, CaC_2, CdI_2, Non ionic crystals – SiC, (BN), crystal composed of discrete molecules

SECTION B

Defect structures: Thermodynamic defects and their consequences, solid electrolytes, non-stoichiometric compounds, F-centres and their applications in non-stoichiometric compounds; Methods to synthesize solid state materials: Ceramic methods, solid state reaction and its kinetics, hydrothermal, sol-gel, co-precipitation (precursor) methods

SECTION C

Amorphous inorganic materials: Glasses, refractories, materials obtained from organometallic chemical vapor deposition (MOCVD); New materials: Conducting polymers, carbon nanotubes, carbon nanorods and fullerenes; Electronic materials: Insulating, semi-conducting and superconducting materials, Ferroelectrics and dielectrics

SECTION D

Intercalation Chemistry: Introduction, intercalation reactions in graphite, layered double hydroxides, layered sulfides, applications of intercalation chemistry; Mesoporous materials and their catalytic applications: Various types of mesoporous materials (oxides, sulphides), tailoring of pore size, applications of mesoporous materials in heterogeneous catalysis

Recommended Books

1. L. E. Smart, E. A. Moore; Solid State Chemistry: An Introduction, 4th ed. CRC Press, 2012

2. A. R. West; Solid State Chemistry and its Applications, 2nd ed. John Wiley, 1990
3. C. N. R. Rao and J. Gopalakrishnan; New Directions in Solid State, Chemistry, 2nd ed. Cambridge University Press, Cambridge, 2002
4. B. E. Douglas, D. H. McDaniel and J. J. Alexander; Concepts and Models of Inorganic Chemistry, 3rd ed. John Wiley & Sons, Inc., New York, 1998

Course Title/Code	Metal clusters and advanced coordination chemistry (CHH632)
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart the knowledge of metal clusters and coordination chemistry related to complex systems
Outcome	Students shall be able to learn the facts of the coordination chemistry, energy level splitting in terms
Prerequisites	Inorganic Chemistry I and II

SECTION-A

Chemistry of Inorganic rings, Cages and metal clusters compounds, borazines, phosphazenes, polyhedral boranes, carboranes, metalloboranes and metallocarboranes

Silicates and aluminosilicates – classifications, structure, properties and applications of naturally occurring silicates and aluminosilicates

SECTION B

Synthesis of Pillared clays and Zeolites

Characterization of clays, pillared clays and Zeolites from measurement of surface area, surface activity pore size, distribution and interlayer spacing

Application of clays, pillared clays and Zeolites with emphasis of catalysis

SECTION C

Introduction to Supramolecular chemistry: Crown ethers, Cryptands, Cyclodextrins and cyclophanes, synthesis of compounds containing new or modified micro cyclic polydentate ligands as well as main group cage and ring compounds, Molecular clefts, tweezers and devices, self assembly and replication

SECTION D

Coordination chemistry: The energy terms, coupling schemes (Russel-Saunders coupling scheme and J-J coupling scheme), Quantitative basis (r, Θ, ϕ) for the splitting of d orbital and energy terms to e_g and t_{2g} in terms of D_q, multielectron systems – the weak and strong filed cases, splitting of term symbols due to spin orbit coupling for a d^1 to d^9 case.

Recommended Books

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. John Wiley & Sons, 2000
2. B. E. Douglas, D. H. McDaniel and J. J. Alexander; Concepts and Models in Inorganic Chemistry, 3rd ed. John Wiley & Sons, 1994
3. B. N. Figgis and M. A. Hitchman; Ligand Field Theory and Its Applications, Wiley Eastern Ltd, 2000
4. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry Principle of Structure and Reactivity, 4th ed. Pearson Education, Inc, 1996
5. P. Atkins, T. Overton, J. Rourke, W. Mark and F. Armstrong; Shriver and Atkins' Inorganic Chemistry, 4th ed. Oxford University Press, 2014

Laboratory IV

Course Title/Code	**LABORATORY WORK-III (CHH633)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-6-0
Objectives	To familiarize with synthesis of Inorganic compounds
Outcome	The student will be able to understand isolation of natural products
Prerequisites	Inorganic Chemistry-I & II

List of Experiments

1. Quantitative separations and determinations of following pairs of metal ions using gravimetric and volumetric methods
    a) Ag+/Cu2+
    b) Cu2+/Zn2+
    c) Fe3+/Ca2+
    d) Ba2+/Cu2+
    e) Ni2+/Zn2+
    f) Ag+/Ni2+
    g) Fe3+/Ni2+
2. Inorganic Preparations of the following compounds
    a) Prussian Blue
    b) Tris acetylacetonato Iron (III)
    c) Tetraammine copper (II) sulphate monohydrate
    d) Hexamine cobalt (III) hexanitrito cobaltate (III)
    e) Sodium hexanitrito cobaltate (III)

Books Recommended

1. J. Singh, R. K. P. Singh, J. Singh, L. D. S. Yadav, I. R. Siddiqui and J. Srivastava; Advanced Practical Chemistry, 2nd ed. Pragati Prakashan, 2010
2. A. I. Vogel; Vogel's textbook of Practical Inorganic Analysis, 5th ed. Longman Scientific and technical Publisher, UK, 1989

Semester III

Elective Courses

Course title/code	**ORGANOMETALIC CHEMISTRY OF TRANSITION METALS AND BIO INORGANIC CHEMISTRY (CHH617)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Elective 4-0-0-0
Objectives	Student will understand the synthesis of π-Complexes of unsaturated Molecules and metal carbonyls. Student will understand the synthesis of Transition Metal Compounds in Homogeneous Catalysis System Student will be exposed to role of metal ions in various biological systems and understand the role of various bio-inorganic molecules in therapeutic use.
Outcome	The student will be able to write the synthesis of π-Complexes of Unsaturated Molecules The student will be able the understand the use of Transition Metal Compounds in Homogeneous Catalysis and biological systems
Prerequisites	Organic Chemistry and Inorganic chemistry-I & II

SECTION A

METAL CARBONYLS: Semibridging carbonyl group; metal nitrosyl carbonyls; tertiary phosphines and arsines as ligands; carbenes and carbynes.

Π-COMPLEXES OF UNSATURATED MOLECULES: Preparation, bonding and structures of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis.

SECTION B

COMPOUNDS OF TRANSITION METAL-CARBON MULTIPLE BONDS Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis Transition Metal Compounds with Bonds to Hydrogen. **TRANSITION METAL Π –COMPLEXES:** Transition metal π -complexes with unsaturated organic molecules , alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

SECTION-C

CATALYSIS: Transition metal ion catalysis for organic transformations and their application in hydrogenation (using symmetric and chiral catalysts), isomerization, olefin oxidation, carbonylation and polymerization reactions. Role of metal ions in biological systems.

SECTION-D

BIO-INORGANIC PROCESSES: Toxic metal ions and their detoxification, chelation therapy/chelating agents in medicine. Recent advances in cancer chemotherapy using chelates. Biological nitrogen

fixation. Natural and synthetic oxygen carriers. Na-K, ATPase or sodium pump. Futuristic aspects of organo transition metal complexes as catalysts and in bio-inorganic chemistry.

Books Recommended

1. F. A. Cotton and G. Wilkinson; Advanced Inorganic Chemistry, 6th ed. John-Wiley & Sons, New York, 1999
2. J. E. Huheey; Inorganic Chemistry, 4th ed. Addison Wesley Pub Co, New York, 1993
3. R. H. Crabtree; The Organometallic Chemistry of the Transition Metals, 1st ed. John-Wiley & Sons, New York, 1988
4. J. P. Collman, L. S. Hegedus, J.R. Norton and R. G. Finke; Principles and Applications of Organotransition Metal Chemistry, 1st ed. University Science Books, Mill Valley, California, 1987
5. M. N. Hughes; The Inorganic Chemistry of Biological Processes, 2nd ed. Wiley, 1981

Course title/code	**Drug Design and Drug Discovery (CHH618)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Elective 4-0-0-0
Objectives	To familiarize with Principles of Drug design and drug discovery To impart knowledge on Quantitative Structure- Activity Relationship (QSAR) studies
Outcome	Students will be able to understand Principles of Drug design and drug discovery The student would be to understand Quantitative Structure- Activity Relationship (QSAR) studies and Combinatorial Synthesis
Prerequisites	Organic Chemistry-I & II

SECTION-A

PRINCIPLES OF DRUG DESIGN AND DRUG DISCOVERY

Introduction to drug discovery: Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries, Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics, Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation, Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine, Discovery of lead structure from natural hormones and neurotransmitters, Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples, Principles of prodrug design, Introduction to drug patents and Clinical trials.

SECTION-B

LEAD MODIFICATION AND SAR STUDIES

SAR: Lead modification strategies, Bioisosterism, variation of alkyl substituents,chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring

contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead.Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs, OC-26: Lead modification and SAR Studies

SECTION-C

QUANTITATIVE STRUCTURE- ACTIVITY RELATIONSHIP (QSAR) STUDIES

Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft's constant, linear and nonlinear relationship between biological activity and Hammett/ Lipophilicity Substituent constants, Lipenski rule of five. Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis, three case studies. Principles of molecular modeling in drug design.

SECTION-D

COMBINATORIAL SYNTHESIS INTRODUCTION: Combinatorial approach, Combinatorial libraries, technologies. Solid phase synthesis, types of resins. Linkers, Reactants for solid phased synthesis, Methods of Parallel synthesis: Haughton's tea bag procedure, Automated parallel synthesis, Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolutionr ecursive deconvolution, tagging and use of decoded sheets, Examples of Combinatorial Chemistry, Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules, Automation in Combinatorial chemistry, High throughput screening.

Books Recommended

1. E. W. Manfred; Burger's medicinal chemistry and drug discovery, Vol V, 6th ed. John wiley Publications, 1995
2. G. L. Patrick and J. Spencer; Introduction to Medicinal chemistry, 6th ed. Oxford University Press, 1995
3. R. B. Silverman and M. W. Holladay, The Organic Chemistry of Drugn design and Drug action, 2nd ed. Academic Press, 2014

Course Title/Code	**Polymer Chemistry (CHH631)**
Course Type	Elective
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart the knowledge of polymer, their processing and characterization
Outcome	Students will be able to learn the application of polymer processing in various fields especially in nanoscience
Prerequisites	Organic and Inorganic Chemistry I and II

SECTION-A

Introduction to polymer science: Nomenclature of polymers, classifications of polymers, applications of polymers

SECTION B

Methods of Polymerization: Step polymerization (Kinetics, molecular weight control in linear polymerization, process conditions, multichain polymerization, cross linking, step co-polymerization), Radical Chain polymerization (kinetics, effect of pressure, process conditions), Ionic chain polymerization (cationic and anionic polymerization of C=C), other polymerization methods

SECTION C

Co-polymerization, polymer characterization, processing and testing of polymers, polymer solutions, measurement of molecular weight and size, structure and properties

SECTION D

Properties of Commercial polymers (Hydrocarbon polymers, Elastomers, Inorganic and Organometallic polymers, Dendritic polymers), and their applications, Polymers Composites, Fibers, High Performance polymers

Recommended books

1. P. J. Flory; Principles of Polymer Chemistry, 1st ed. Cornell University Press, 1953
2. F. W. Billmeyer; Polymer Chemistry, 1st ed. John-Wiley & Sons, 1971
3. H. R. Alcock and F. W. Lambe; Contemporary Polymer Chemistry, Prentice Hall, 1996
4. V. R. Gowarikar, N. V. Visvanathan and J. Sreedhar; Polymer Science, Wiley Eastern, 1986
5. G. Odean; Principles of Polymerization, 4th ed. McGraw Hill Book Company, New York, 2004

Semester IV

(Organic Specialization)

Organic Specialization
SEMSETER IV

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core(Departmental/Allied)/ Elective (Departmental/ Open) / University Compulsory	Hard/Soft/ Workshop/ NTCC	L	T	P	O		
CHH623	ADVANCED HETEROCYCLIC CHEMISTRY	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH624	CHEMISTRY OF NATURAL PRODUCTS	CORE (Departmental)	HARD	4	0	0	0	4	4
CHH625 CHH626	ELECTIVE-II (A) BIOORGANIC CHEMISTRY (B) GROUP THEORY AND ITS APPLICATIONS (C) NANOSCALE MATERIALS: SYNTHESIS, PROPERTIES AND APPLICATIONS	ELECTIVE (Departmental)	HARD	4	0	0	0	4	4
CHH627	LABORATORY WORK-V	CORE (Departmental)	HARD	0	0	6	0	6	3
CHN628	PROJECT WORK	CORE (Departmental)	NTCC	0	0	0	6	6	6

DETAILED SYLLABUS
CHP01 –FOURTH SEMESTER

Course Title/Code	**ADVANCED HETEROCYCLIC CHEMISTRY (CHH623)**
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge on synthesis of Five and six- member heterocyclic compounds with two or more hetero atoms To familiarize with the synthesis of larger ring heterocyclic compounds
Outcome	Students will be able to write the synthesis of Five and six- member heterocyclic compounds with two or more hetero atoms Students will be able to write the synthesis of larger ring heterocyclic compounds
Prerequisites	Organic Chemistry-I & II

SECTION-A

NON-AROMATIC HETEROCYCLICS: Different types of strains, interactions and conformational aspects of nonaromatic heterocycles viz. cyclopropane , cyclobutane. Synthesis, reactivity and importance of the following ring systems, Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines and Oxetanes

SECTION-B

FIVE AND SIX MEMBERED HETEROCYCLICS WITH TWO HETERO ATOMS: Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole**.**

SECTION-C

HETEROCYCLICS WITH MORE THAN TWO HETERO ATOMS: Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoies,1,2,4-triazoles,Tetrazoles, 1,2,4-oxadiazole, 1 ,3,4-oxadiazole, 1,2,5- oxadiazole, 1,2,3-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5-thiadiazoles, 1,2,3-triazine, 1,2,4- triazine, 1,3,5- triazine, tetrazines. Synthesis and importance of purines. Syntheis of Caffeine, theobromine and theophylline.

SECTION-D

LARGER RING AND OTHER HETEROCYCLES: Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepines. Synthesis of Diazepines rearrangements of 1,2 - diazepines. Synthesis of

Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.

Books Recommended

1. T. Gilchrist; Heterocyclic Chemistry, 3rd ed. Addison-Wesley Longman Ltd, London, 1998
2. R. M. Acheson; An introduction to the Chemistry of heterocyclic compounds, 2nd ed. Interscience, 1960
3. J. A. Joule and K. Mills; Heterocyclic Chemistry; 3rd ed. Chapman and Hall, 1995
4. L. A. Paquette; Principles of Modern Heterocyclic Chemistry, W. A. Benzamin, 1968
5. A. R. Katritzky; Handbook of Heterocyclic Chemistry, 3rd ed. Pergamon Press, 1976

Course Title/Code	CHEMISTRY OF NATURAL PRODUCTS (CHH624)
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge on Biosynthesis of natural products.To familiarize with Structure determination and stereochemistry of natural products by chemical methods and spectroscopic methods
Outcome	Students will be able to write Biosynthesis of natural products.Students will be able elucidate the structure of natural products by various spectroscopic techniques
Prerequisites	Nil

SECTION-A

Biosynthesis of secondary metabolites: Introduction to natural products, Synthesis and Biosynthesis (similarities & differences), Biogenesis, Primary and secondary metabolites, Why plant produce secondary metabolites, Charecteristics of secondary metabolites, Biosynthesis of natural products (schematic representation), methods of investigation of biosynthesis of secondary metabolites, Reactions involve in biosynthesis (primary and secondary biosynthesis);

Biosynthesis of Acetyl CoA: biosynthesis by oxidative decarboxylation, Activation of acetic acid, properties (formation of malonyl CoA); Origin of aromatic ring in secondary metabolites (Shikimic acid pathway); Biosynthesis of terpenes (NPP, GPP, citral, α-pinene, α-terpineol, borneol); Biosynthesis of steroids (cholesterol), Biosynthesis of alkaloids: formation of alkaloid derived from phenylalanine-ephedrine, Biosynthesis of piperdine alkaloid-coniine, biosynthesis of pyrrolidine-pyridine alkaloid-nicotine, biosynthesis of tropane alkaloid-atropine, biosynthesis of cinchona alkaloid-quinine. Biosynthesis of fatty acids

SECTION-B

Terpenoids & Carotenoids:

Terpenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Isolation of terpenes, Structure determination,

Monoterpenoids: Citral, geraniol (acyclic), α-terpeneol, menthol (monocyclic).
Sesquiterpenoids: Farnesol (acyclic), zingiberene (monocyclic), santonin (bicyclic),
Diterpenoids: Phytol and abietic acid.

Carotenoids: General methods of structure determination of Carotenes: β- carotene, lycopene

SECTION-C

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 and synthesis of the following: Ephedrine, Coniine, Nicotine, Atropine, Quinine and Morphine.

SECTION-D

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Androsterone, Testosterone, Progestrone.

Plant Pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Anthocyanins (Cyanin and pelargonidin), polyphenols: Flavones (chrysin), Flavonols (quercitin) and isoflavones (daidzein) coumarin, Quinones (lapachol), Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

Books Recommended:

1. J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthrope and J. B. Harborne; Natural Products-Chemistry and Biological Significance, 1st ed. Longman group U. K. limited, Essex, 1994
2. I. L. Finar; Organic Chemistry, Vol. II, 5th ed. Pearson Education, 1956
3. M. Nogradi; Stereo selective synthesis- A Practical Approach, 2nd ed. Wiley-VCH, 1994
4. K. Hostettmann, M. P. Gupta and A. Marston; Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Harwood Academic Publishers, 1999

Course Title/Code	**LABORATORY WORK-V (CHH627)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-6-0
Objectives	To familiarize with synthesis of drugs in laboratory To impart knowledge on estimation of drugs.
Outcome	Students will be able to understand synthesis of drugs in laboratory and their estimation.
Prerequisites	Organic Chemistry-I & II

LIST OF EXPERIMENTS

LABORATORY SYNTHESIS OF THE FOLLOWING ORGANIC COMPOUNDS

1. Phenyl acetate
2. Mannitol Hexa-acetate
3. P-amino azo benzene from aniline
4. Anthranilic acid from phthalic anhydride
5. P-nitro aniline from acetanilide

Other organic preparation of one step, two step or three step synthesis

Books Recommended

1. F. G. Mann and B. C. Saunders; Practical organic chemistry, 4th ed. Longman Scientific and technical Publisher, UK, 1936

2. A. I. Vogel; Vogel's textbook of Practical Organic Chemistry, 5th ed. Longman Scientific and technical Publisher, UK, 1989

Course Title/Code	**Project Work (CHN628)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-0-6
Objectives	To make the students understand and analyze the specific problem To plan the experimental work and analyze the results To compile the data and prepare the project report

Semester IV

(Inorganic Specialization)

SEMSETER IV

COURSE CODES	COURSE NAME	COURSE TYPE	COURSE NATURE	PERIODS				NO. OF CONTACT HOURS PER WEEK	CREDITS
		Core(Departmental/ Allied)/ Elective (Departmental/ Open) / University Compulsory	Hard/Soft / Workshop / NTCC	L	T	P	O		
CHH634	APPLIED ORGANOMETALLIC AND APPLIED BIO-CATALYSIS	CORE(Departmental)	HARD	4	0	0	0	4	4
CHH635	NUCLEAR, RADIOCHEMISTRY AND LASERS	CORE(Departmental)	HARD	4	0	0	0	4	4
CHH625 CHH626 CHH636	ELECTIVE-II (A) BIOORGANIC CHEMISTRY (B) GROUP THEORY AND ITS APPLICATIONS (c) NANO SCALE MATERIALS: SYNTHESIS, APPLICATION AND PROPERTIES	ELECTIVE (Departmental)	HARD	4	0	0	0	4	4
CHH637	LABORATORY WORK-V	CORE(Departmental)	HARD	0	0	6	0	6	3
CHN628	PROJECT WORK	CORE(Departmental)	NTCC	0	0	0	6	6	6

DETAILED SYLLABUS

Semester IV

Course Title/Code	**Nuclear, Radio and Laser Chemistry (CHH635)**
Course Type	Elective
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge about the nuclear reactions, nuclear energy and its applications
Outcome	Students shall be able to learn about the various fields of nuclear reactions
Prerequisites	Inorganic Chemistry I and II

SECTION-A

Nuclear reactions: types of reactions, Production of projectiles, nuclear cross-sections, chemical effects of nuclear transformation, Q value, Natural and artificial radioactivity, radioactive decay and equilibrium, interactions of nuclear radiations with matter, Nuclear fission-fission product and fission yields, Nuclear fusion, Binding energy and stability, empirical mass equation, Hot atom chemistry, Radiation hazards and therapeutics, detectors and their principles, the direction of radiochemistry

SECTION B

The nuclear models, the liquid drop model, the shell model, the Fermi gas model & collective nuclear model, nuclear spin, parity & magnetic moments of odd mass numbers nuclei

Nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions

SECTION C

Systematic of alpha, beta and gamma decays: Alpha decay, energy curve, spectra of alpha particles, Giger-Nuttal law, theory of alpha decay, penetration of potential barrier, beta decay, range of energy relationship, beta spectrum, sergeants curve, Fermi theory of beta decay, matrix elements, allowed and forbidden transitions, curie plots, gamma decay, Nuclear energy levels, selection rule, isomeric transitions, Internal conversion, Auger effect.

Radioactive techniques: Tracer technique, (neutron activation analysis), Counting techniques such as G.M. Ionization and proportional counters.

SECTION D

Lasers Chemistry: Einstein's equation of absorption and emission of electromagnetic radiation with reference to lasers, induced emission, stimulated emission, laser action, populated inversion, pump radiation, light amplification, properties of laser, single mode, CW and mode locked lasers, Gas lasers, solid state lasers, Applications of lasers to the study of chemical reactions

Recommended Books

1. G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller; Nuclear and Radiochemistry, Wiley Interscience, 1981
2. W. D. Ehmann and D. E. Vance; Radiochemistry and Nuclear Methods of Analysis, Wiley Interscience, 1991
3. B.G. Harvey; Introduction to Nuclear Physics and Chemistry, 2nd ed. Prentice hall, 1969
4. H. J. Arnikar; Essentials of Nuclear Chemistry, 2nd ed. John Wiley, 1994
5. B.K. Sharma; Nuclear and Radiation Chemistry, Krishna Publication, 2011

Course Title/Code	**Applied Organometallic and Applied Biocatalysis (CHH634)**
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge about the advanced Organometallic Chemistry and biocatalysis
Outcome	Students shall be able to learn about the concepts of advanced organometallic chemistry and biocatalysis
Prerequisites	Organometallic Chemistry and coordination Chemistry

SECTION A

Introduction to homogeneous catalysis, TON and TOF, some aspects of commonly used ligands in homogeneous catalysis such as CO, amines, phosphines, NHC's, alkenes, alkynes, carbenes, carbines, etc. Recent developments in hydrogenation and hydroformylation and their asymmetric variations using OM catalysts

SECTION B

Wacker's oxidation, Monsanto and Cativa processes, Olefin and alkyne trimerization and oligomerization, Olefin polymerization using Ziegler-Natta, Titanium group metallocenes, post metallocenes late TM catalyst and FI catalysts, Olefins and alkyne metathesis, Grubbs I, II and III, Schrock and Schrock-Hoveyda catalysts, types of metathesis such as RCM, ROM, ROMP, ADMET and EM

SECTION C

Applications in Industry, Palladium and Nickel catalyzed cross coupling reactions such as Ssuzuki, Heck, Sonogashira, Stille, Negishi, Hiyama, Buchwald-Hartwig, decarboxylative cross coupling and

alpha arylation of carbonyls, Fischer Tropsch process, C-H activation of alkyls and aryls suing transition metal complexes

SECTION D

Introduction to enzymes and enzyme catalysed reactions, classification and mechanisms of reaction, purification and characterization of enzymes, Michelis Menten Kinetics, Industrial enzymes, applications of enzymes in diagnostics, analysis, biosensors, biotransformations, enzyme structure determination, stability, stabilization, enzyme immobilization and concept of enzyme engineering, nano-biocatalysis

Recommended Books

1. R. H. Crabtree; The Organometallic Chemistry of the transition metals, 5th ed. Wiley Publication, 2009
2. A. Elias and B. D> Gupta; Basic Organometallic Chemistry, 2nd ed. Oxford University Press, 2013
3. Coates; Principles of Organometallic Chemistry, Springer Verlag Publisher, 1968

Course Title/Code	**LABORATORY WORK-III (CHH637)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-6-0
Objectives	To familiarize with synthesis of Inorganic compounds
Outcome	The student will be able to understand isolation of natural products
Prerequisites	Inorganic Chemistry-I & II

List of Experiments

1. Determination of Ca^{2+} and Mg^{2+} ions through EDTA titrations
2. Separation of zinc and magnesium on an ion exchanger
3. Determination of hydrazine titrimetrically
4. Preparation of biguanide
5. Quantitative separations and determinations of following pairs of metal ions using gravimetric and volumetric methods
    a) Ca2+/Mg2+
    b) Ag+/Cu2+
    c) Pb2+/Cu2+
6. Separation of Ions using chromatography
    a) Paper chromatography separation of Ag+, Pb2+, Hg2+ ions
    b) Paper chromatography separation of Ni3+, Co2+, Zn2+, ions
    c) Paper chromatography separation of Ba2+, Sr2+ and Ca2+ ions

Recommended Books

1. J. Singh, R. K. P. Singh, J. Singh, L. D. S. Yadav, I. R. Siddiqui and J. Srivastava; Advanced Practical Chemistry, 2nd ed. Pragati Prakashan, 2010
2. A. I. Vogel; Vogel's textbook of Practical Inorganic Analysis, 5th ed. Longman Scientific and technical Publisher, UK, 1989

SEMESTER IV

Electives

Course Title/Code	BIOORGANIC CHEMISTRY (CHH625)
Course Type	Core
Course Nature	Elective
L-T-P-O Structure	4-0-0-0
Objectives	To familiarize with mechanism of enzymatic reactions. To impart knowledge on various enzymatic Models and transformation reactions To impart basic knowledge on Fermentation technology and genetic engineering
Outcome	Students would be able to understand various enzymatic models Students would be able to write various transformation reactions Students will be able to understand the basics of Fermentation technology and genetic engineering
Prerequisites	Organic Chemistry-I & II

SECTION-A

ENZYMES AND THEIR ACTION

Introduction to enzymes. Transition state theory,Acid-Base catalysis, Covalent catalysis— Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. Examples of some typical enzyme mechanisms for (1) Triose phosphate isomerase, (ii) α-chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease..

SECTION-B

ENZYME MODELS AND ENZYMATIC TRANSFORMATIONS

Introduction — Biomimetic chemical approach to biological systems-Enzyme models Advantage of enzyme models. Requirements necessary for the design of enzyme models, Host-Guest complexation chemistry. Examples of some host molecules-Crown ether cryptanes, cyclodextrins, Cyclodextrin based enzyme models-Valixarenes, ionophores, micelles and synzymes (synthetic enzymes) — chiral recognition and catalysis.Introduction to industrial enzymes, Enzymatic synthesis of α-amino acids and peptides, Transformations of lipases and esterases, Kinetic resolutions of catboxylic acids, esters and alcohols – Transesterification, Amine resolution-use of oxido-reductase, C-C bond formation using enzymes-asymmetric cyanohydrin formation and asymmetric aldol condensations.

SECTION-C

RECOMBINANT DNA AND FERMENTATION TECHNOLOGY

Introduction to genetic engineering. Recombinant DNA technology-restriction endonuclease, cloning, linkers, adaptors, Application of recombinant DNA technology in production of

pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples, Principles of finger printing technology- Site directed mutagenesis. **FERMENTATION TECHNOLOGY:** Introduction to fermentation. Industrial fermentation, Advantages and limitations of fermentation, Production of drugs and drug intermediates from fermentation examples, Chiral hydroxy acids, vitamins, amino acids, β-lactam antibiotics, Precursor fermentation and microbial oxidation and reductions.

SECTION-D

COENZYMES: Introduction, Co factors — cosubstrates — prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP+ NADPH) ii) Flavin adenine nucleotide FAD, $FADH_2$ and iii) Flavin mononucleotide (FMN, FMNH2) lipoicacid, biotin, tetrahydrofolate and ubiquinone, Adenosine triphosphate ($_{ATP}$) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphospho sugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

Recommended Books

1. C. F.A. Bryce, K. Jayaraman, J. Green, K. Dharmalingam and D. Balasubramananian; Concepts in biotechnology, University Press, 2004
2. H. R. Horton; Principals of biochemistry, 18th ed. Pearson Prentice Hall, 2006
3. H. Dugas and C. Penney; Bioorganic chemistry - A chemical approach to enzyme action, Vol II, Springer Verlag, 1981

Course Title/Code	**GROUP THEORY AND ITS APPLICATIONS (CHH626)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Elective 4-0-0-0
Objectives	To familiarize with Symmetry elements and symmetry operations To impart knowledge on optical activity
Outcome	Students will be able to understand group representation of various molecules.
Prerequisites	Organic Chemistry-I & II

Section A

MOLECULAR SYMMETRY: Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation.Products of symmetry operations, equivalent atoms and equivalent symmetry elements, relations between symmetry elements and operations, classes of symmetry operations, point groups and classification.Symmetry: Optical activity and dipole moment

Section B

REPRESENTATION OF GROUPS: Reducible and irreducible representations. The great Orthogonality theorem, character tables, position vector and base vector as basis for representation.Wavefunctions as bases for irreducible representations (p an d-orbitals). Direct product. Vanishing integral.

Section C

COUPLING FOR TRANSITION METALS: Russell-Saunders coupling for d_n method of states. Splitting of one-electron levels in an octahedral environment. Correlation diagram. The method of descending symmetry, selection rules, Application of group theory to chemical bonding, hybridizations

Section D

APPLICATION OF GROUP THEORY: Applications of group theory in Vibrational Spectroscopy: A brief idea about Infrared and Raman scattering spectroscopy. Vibrational modes as basis of group representations, Mutual exclusion principle, Classification of vibrational modes (i.e. stretching and angle deformation vibrations)

Books Recommended

1. F. A. Cotton; Chemical applications of Group Theory, 2nd ed. John Wiley & Sons, 1971
2. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Longman, 1962
3. V. H. H. Jaffe and M. Orchin; Symmetry in Chemistry, John Wiley & Sons, New York, 1965

Course Title/Code	**Nanoscale materials: Synthesis, Properties and Applications (CHH636)**
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge about the nanoscale materials: its uses and applications in various fields
Outcome	Students shall be able to learn about the use of nanoscale materials
Prerequisites	Inorganic Chemistry I and II

SECTION A

Introduction to nanoscale materials: The nano-length scale, quantum confinement effect, conceptual development of band theory – from molecules to clusters/quantum dots to macroscopic crystals, material dependence of nanoscale and quantum size-effect, crystalline and amorphous nanomaterials, nanocrystals, surface energy and crystal facets

SECTION B

Properties of nanomaterials: Surface area measurement, determination of size and textural studies, composition and elemental analysis, high chemical reactivity of nanoscale materials, effect of size and shape on nanocrystal reactivity, agglomeration and sintering of nanomaterials, dispersibility and chemical stability of nanoparticles in solution, Surface Plasmon resonance, surface modification of metallic and semiconductor nanoparticles, nanofabrication and nano-manipulations

SECTION C

Synthesis of nanomaterials: Concepts of top-down and bottom-up approaches, chemical, aero-gel, aerosol, spray-pyrolysis, micro-emulsion, solvo thermal, sonochemical, chemical and microwave methods of synthesis of nanoparticles,

Toxicity of nanomaterials: Health concerns of using nanomaterials, inhalation toxicity, oral toxicity, environmental toxicity, cyto- and bio-toxicity of nanomaterials, environmental protection and precautions

SECTION D

Applications of Nanoparticles: Biocidal applications of nanomaterials, metal oxides nanoparticles and their application in photo electronic splitting of water, application of nanomaterials in medicinal fields; Carbon nanotubes: sensing applications, single molecule memory devices, electronic and optoelectronic applications, transistors for digital electronics; Graphene: sensing application, graphene transistor, –electronics and optoelectronics, digital electronics, photovoltaics; Polymer and carbon nanotube composites for space applications: meteoroids, micrometeoroids, and space-debris, conductive coatings for electrostatic discharge, thermal conductivity, space elevator, solar sails

Recommended Books

1. K. J. Klabunde; Nanoscale Materials in Chemistry, 2nd ed. Wiley- Interscience, New York, 2001
2. G. Schmid; Nanoparticles: From Theory to Application, 6th ed. Wiley- VCH, Weinheim, 2004
3. G. Cao and Y. Wang; Nanostructures and Nanomaterials: Synthesis, Properties and Applications, 2nd ed. World Scientific, 2004
4. C. N. R. Rao, A. Müller and A. K. Cheetham; The Chemistry of Nanomaterials: Synthesis, Properties and Applications, Vol. I & II, Wiley-VCH Verlag, Weinheim, 2004
5. J. A. Rodriguez and G. M. Fernandez; Synthesis, Properties and Applications of Oxide Nanomaterials, John Wiley, New York, 2007