MANAV RACHNA UNIVERSITY

FACULTY OF APPLIED SCIENCES

DEPARTMENT OF CHEMISTRY

PROGRAM STRUCTURE

&

DETAILED SYLLABUS

M.Sc. Chemistry

BATCH: 2019-2021

MANAV RACHNA UNIVERSITY
DEPARTMENT OF CHEMISTRY
M.SC (CHP01)
SCHEME-B (Effective from July 2019)

SEMESTER-1

SUBJECT CODES	SUBJECT NAME	OFFERING DEPARTMENT	COURSE NATURE (Hard/Soft/ NTCC)	COURSE TYPE (Core/ Elective etc)	L	T	P	O	CONTACT HOURS PER WEEK	NO. OF CREDITS
CHH501B	Physical Chemistry-I	CH	Hard	Core	4	0	0	0	4	4
CHH502B	Inorganic Chemistry-I	CH	Hard	Core	4	0	0	0	4	4
CHH503B	Organic Chemistry-I	CH	Hard	Core	4	0	0	0	4	4
CHH504B	Analytical Chemistry	CH	Hard	Core	4	0	0	0	4	4
CHH505B	Laboratory-I	CH	Practical	Core	0	0	12	0	12	6
	Total (L-T-P-O/Contact Hours/Credits)				16	0	12	0	28	22

SEMESTER - 2

SUBJECT CODES	SUBJECT NAME	OFFERING DEPARTMENT	*COURSE NATURE (Hard/Soft/ NTCC)	COURSE TYPE (Core/ Elective etc)	L	T	P	O	CONTACT HOURS PER WEEK	NO. OF CREDITS
CHH506B	Physical Chemistry-II	CH	Hard	Core	4	0	0	0	4	4
CHH507B	Inorganic Chemistry-II	CH	Hard	Core	4	0	0	0	4	4
CHH508B	Organic Chemistry-II	CH	Hard	Core	4	0	0	0	4	4
CHH509B	Molecular Spectroscopy	CH	Hard	Core	4	0	0	0	4	4

CHH510B	Laboratory-II	CH	Practical	Core	0	0	8	0	8	4
RDO503	Scientific Research-I	CH	NTCC	Core	0	0	0	4	2	4
	Total (L-T-P-O/Contact Hours/Credits)				16	0	8	4	26	24

SEMESTER - 3

SUBJECT CODES	SUBJECT NAME	OFFERING DEPARTMENT	*COURSE NATURE (Hard/Soft/ NTCC)	COURSE TYPE (Core/ Elective etc)	L	T	P	O	CONTACT HOURS PER WEEK	NO. OF CREDITS
CHH 601B	Symmetry & Group Theory	CH	Hard	Core	4	0	0	0	4	4
CHH 602B	Physical Special-I (Magneto-chemistry, Chemical Kinetics, Catalysis & ion transport)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 608B	Inorganic Special-I (Organometalic Chemistry of Transition Metals & Bio Inorganic Chemistry)									
CHH613B	Organic Special-I (Statistical Stereochemistry & Asymmetric Synthesis)									
CHH 603B	Physical Special-II (Irreversible thermodynamics, Transport Phenomenon, Photochemistry & Fast Reaction)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 609B	Inorganic Special-II (Supramolecular Chemistry & Metal Clusters)									
CHH614B	Organic Special-II (Photochemistry & Pericyclic Reaction)									

CHH 604B / CHH 605B	Physical Elective:(Advanced Spectroscopy/ Advanced Chemical Kinetics)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 610B/ CHH 611B	Inorganic Elective: (Solid state Materials / Inorganic & Biological Catalysis)									
CHH615B CHH616B CHH617B	(Modern Organic Synthetic Technique / Bioorganic Chemistry/ Chemistry of Natural Products)									
CHH 606B	Physical Laboratory	CH	Practical	Core	0	0	8	0	8	4
CHH-612B	Inorganic Laboratory									
CHH-618B	ORGANIC LABORATORY WORK									
RDO603	Scientific Research-II	CH	NTCC	Core	0	0	0	4	2	4
	Total (L-T-P-O/Contact Hours/Credits)				16	0	8	4	26	24

SEMESTER - 4

SUBJECT CODES	SUBJECT NAME	OFFERING DEPARTMENT	COURSE NATURE (Hard/Soft/ NTCC)	COURSE TYPE (Core/ Elective etc)	L	T	P	O	CONTACT HOURS PER WEEK	NO. OF CREDITS
CHN619B	MAJOR PROJECT (Industrial or research lab training)	CH	NTCC	CORE	0	0	0	12	0	12
	TOTAL (L-T-P-O/CONTACT HOURS/CREDITS)				0	0	0	12	0	12

Semester	Classroom Contact hours	Non teaching Outcome hrs	credits
FIRST SEMESTER	28	0	22
SECOND SEMESTER	26	4	24
THIRD SEMESTER	26	4	24
FOURTH SEMESTER	0	12	12
TOTAL	80	20	82

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

MANAV RACHNA UNIVERSITY
FACULTY OF APPLIED SCIENCES
DEPARTMENT OF CHEMISTRY
M.SC. (2019-2021)
SYLLABUS & SCHEME
EFECTIVE FROM JULY 2019

(CHP01) SEMSETER I

Subject Codes	Subject Name	Offering Department	Course Nature (Hard/ Soft/ NTCC)	Course Type (Core/ Elective)	L	T	P	O	Contact Hours Per Week	No. Of Credits
CHH 501B	Physical Chemistry-I	CH	Hard	Core	4	0	0	0	4	4
CHH 502B	Inorganic Chemistry-I	CH	Hard	Core	4	0	0	0	4	4
CHH 503B	Organic Chemistry-I	CH	Hard	Core	4	0	0	0	4	4
CHH 504B	Analytical Chemistry	CH	Hard	Core	4	0	0	0	4	4
CHH 505B	Laboratory-I	CH	Practical	Core	0	0	12	0	12	6
	Total (L-T-P-O/Contact Hours/Credits)				16	0	12	0	28	22

SEMESTER II

Subject Codes	Subject Name	Offering Department	Course Nature (Hard/Soft/ NTCC)	Course Type (Core/ Elective)	L	T	P	O	Contact Hours Per Week	No. Of Credits
CHH 506B	Physical Chemistry-II	CH	Hard	Core	4	0	0	0	4	4
CHH 507B	Inorganic Chemistry-II	CH	Hard	Core	4	0	0	0	4	4
CHH 508B	Organic Chemistry-II	CH	Hard	Core	4	0	0	0	4	4
CHH 509B	Molecular Spectroscopy	CH	Hard	Core	4	0	0	0	4	4
CHH 510B	Laboratory-II	CH	Practical	Core	0	0	8	0	8	4
CHN 511B	Scientific Research-I	CH	NTCC	Core	0	0	0	4	2	4
	Total (L-T-P-O/Contact Hours/Credits)				16	0	8	4	26	24

Physical Chemistry Specialization

SEMSETER III

Subject Codes	Subject Name	Offering Deptt.	Course Nature (Hard/Soft/ NTCC)	Course Type (Core/ Elective)	L	T	P	O	Contact Hours Per Week	No. Of Credits
CHH 601B	Symmetry & Group Theory	CH	Hard	Core	4	0	0	0	4	4
CHH 602B	Physical Special-I (Magneto-chemistry, Chemical Kinetics, Catalysis & ion transport)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 603B	Physical Special-II (Irreversible thermodynamics, Transport Phenomenon, Photochemistry & Fast Reaction)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 604B / CHH 605B	Physical Elective: (Advanced Spectroscopy/ Advanced Chemical Kinetics)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 606B	Physical Laboratory	CH	Practical	Core	0	0	8	0	8	4
CHN 607B	Scientific Research-II	CH	NTCC	Core	0	0	0	4	2	4
	Total (L-T-P-O/Contact Hours/Credits)				16	0	8	4	26	24

Inorganic Chemistry Specialization

SEMSETER III

Subject Codes	Subject Name	Offering Deptt	Course Nature (Hard/Soft /Ntcc)	Course Type (Core/ Elective)	L	T	P	O	Contact Hours Per Week	No. Of Credits
CHH 601B	Symmetry & Group Theory	CH	Hard	Core	4	0	0	0	4	4
CHH 608B	Inorganic Special-I (Organometalic Chemistry of Transition Metals & Bio Inorganic Chemistry)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 609B	Inorganic Special-II (Supramolecular Chemistry & Metal Clusters)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 610B/ CHH 611B	Inorganic Elective (Solid state Materials / Inorganic & Biological Catalysis)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 612B	Inorganic Laboratory	CH	Practical	Core	0	0	8	0	8	4
CHN 607B	Scientific Research-II	CH	NTCC	Core	0	0	0	4	2	4
	Total (L-T-P-O/Contact Hours/Credits)				16	0	8	4	26	24

Organic Chemistry Specialization

SEMSETER III

Subject Codes	Subject Name	Offering Deptt	Course Nature (Hard/Soft /NTCC)	Course Type (Core/ Elective)	L	T	P	O	Contact Hours Per Week	No. Of Credits
CHH 601B	Symmetry & Group Theory	CH	Hard	Core	4	0	0	0	4	4
CHH 613B	Organic Special-I (Statistical Stereochemistry & Asymmetric Synthesis)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 614B	Organic Special-II (Photochemistry & Pericyclic Reaction)	CH	Hard	Special Core	4	0	0	0	4	4
CHH 615B /CHH 616B /CHH 617B	Organic Elective (Modern Organic Synthetic Technique / Bioorganic Chemistry/ Chemistry of Natural Products	CH	Hard	Special Core	4	0	0	0	4	4
CHH 618B	Organic Laboratory	CH	Practical	Core	0	0	8	0	8	4
CHN 607B	Scientific Research-II	CH	NTCC	Core	0	0	0	4	2	4
	Total (L-T-P-O/Contact Hours/Credits)				16	0	8	8	26	24

SEMSETER IV

Subject Codes	Subject Name	Offering Department	*Course Nature (Hard/Soft/ NTCC)	Course Type (Core/ Elective Etc)	L	T	P	O	Contact Hours Per Week	No. Of Credits
CHN 619 B	Major Project (Industrial or Research Lab Training)	CH	NTCC	Core	0	0	0	12	0	12
	Total (L-T-P-O/Contact Hours/Credits)				0	0	0	12	0	12

TOTAL CREDITS FOR SEMESTER I –IV

S.No.	Semester	Classroom Contact Hours	Non Teaching Outcome Hrs	Credits
1	First Semester	28	0	22
2	Second Semester	26	4	24
3	Third Semester	26	4	3
4	Fourth Semester	0	12	24
Total Credits For M.Sc. Chemistry Programme		80	30	82

SECTION WEIGHTAGE PARAMETERS

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

SEMESTER I

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: Solutions: Activity coefficients and ion-ion interactions. Physical significance of activity coefficients, mean activity coefficient of an electrolyte and its determination, Derivation of the Debye-Hückel theory of activity coefficients (both point ion size and finite ion size models), Excess functions, Metal/Electrolyte interface: Introduction and characteristics (OHP and IHP, potential profile across double layer region)

SECTION-B

Surface phenomena: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Krafft temperature, Factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellization, solubilization, microemulsions, reverse micelles, surface films (eletrokinetic phenomena), catalytic activity at surfaces. Electrode/ electrolyte interface; Nernst equation.

SECTION-C

Quantum Chemistry: Postulates of Quantum mechanics, Linear and Hermitian operators, Turn-over rule, Commutation of operators and Uncertainty principle. Some exactly soluble problems: Particle in a box (1-D, 2-D & 3-D) and ring. Concept of degeneracy and its application to Jahn-Teller distortion, Simple harmonic oscillator problem and its solution using series solution or factorization method, Calculation of various average values, Brief Description: Angular momentum operators, Eigen values and eigen-functions, Radial distributions.

SECTION-D

Approximate methods: First order time-independent perturbation theory for non-degenerate states, Variation theorem and variational methods, Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, and approximate functions for particle in a box and hydrogen atom).

HMO method and its applications: π-Electron approximation, Huckel Molecular Orbital Theory of conjugated systems Ladder operators and recursion relations of Hermite polynomials, Generating functions, Rodrigues Representation. Derivation of rigid rotator and H-atom (energy quantization)

Books Recommended

1. J. M. Bockris and A. K. N. Reddy, Modern Electrochemistry 1 (Ionics), Springer (2006).
2. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
3. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).
2. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).
3. Mortimer, R. G. Mathematics for Physical Chemistry 2nd Ed. Elsevier (2005).
4. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).
5. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
6. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).

Course Title/Code	**Inorganic Chemistry-I (CHH 502B)**
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, CFT splitting of d orbitals in octahedral, tetrahedral and square planar complexes, factors affecting CFT, CFSE, applications of CFT, Spectrochemical series and effects of covalency. Nephelauxetic series, magnetic properties of transition metal complexes, Jahn-Teller distortions, Jahn Teller stabilization energy; molecular orbital theory of octahedral complexes

SECTION-B

Electronic Spectra Of Transition Metal Complexes: Types of transition, selection rules for electronic transitions and relaxation of selection rules, width of absorption bands, electronic spectra of transition metal complexes, Term-symbols, Russel-Saunders states, Spectroscopic ground states; Coupling schemes, Orgel diagrams,determination of *Dq*and Racah parameters, Charge transfer spectra (MLCT, LMCT).

SECTION-C

Organometallic Chemistry-I: Classification of organometallic compounds, nomenclature, EAN, 18 e rule, reactions: oxidative addition, reductive elimination, insertion; σ bonded organometallic

compounds and Π bonded organometallic compounds, role of organometallic compounds in catalysis (hydrogenation, hydroformylation)

SECTION-D

Metal Carbonyls: Classification of metal carbonyls (mono, bi, poly, bridging), general method of preparation, structure of metal carbonyl, vibrational spectra of metal carbonyls for bonding and structural elucidation (homoleptic and heteroleptic), introduction to tertiary phosphine as ligands.

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 (CHH 503B)**
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To familiarize with reactive intermediates of organic chemistry and its generation. To impart knowledge of Nucleophilic Substitution and reactivity effects of substrate structure To impart knowledge of nucleophilic and electrophilic aromatic substitution reactions To impart the knowledge of neighboring groups effect on product formation
Outcome	Students will be able to understand the concept of reactive intermediate in organic chemistry. Students will be able to grasp in depth knowledge of Nucleophilic and Electrophilic Substitution reactions and its implications on various organic reactions Students will be able to understand the neighboring group effect on product formation
Prerequisites	B.Sc. with Chemistry as one of the Subject

SECTION A

Reactive Intermediates in Organic Chemistry

Carbocations: Classical and non-classical, neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, stability and reactivity of bridge-head carbocations.
Carbanions: Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications.
Free Radicals: Generation, structure, stability and reactions, cage effects; radical-cations & radical anions,
Carbenes: Formation and structure, reactions involving carbenes and carbenoids.
Nitrenes: Generation, structure and reactions of nitrenes.
Arynes: Generation and reactivity of arynes, nucleophilic aromatic substitution reactions, SNAr mechanism; Ipso effect.

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

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	ANALYTICAL CHEMISTRY (CHH 504B)
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

Analytical chemistry and chemical analysis, Classification of analytical methods, Method selection, Sample processing, Steps in a quantitative analysis, Data organization, analytical validations, Limit of detection and limit of quantization.

Atomic Spectroscopy: Atomic absorption (AAS), emission (AES) and inductively coupled plasma (ICP) spectroscopy.

SECTION B

Photoelectron Spectroscopy: Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2, CO, HF, NH_3 and H_2O - ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

SECTION C

Optical Methods: Electronic spin resonance spectra, Mossbauer spectroscopy.

Theory, Instrumentation and applications of X-rays (emission, absorption, diffraction Methods)

Capillary electrophoresis, Potentiometry, Coulometry, Voltametry

SECTION D

Chromatographic Techniques: HPLC, HPTLC and GC its instrumentation, working, applications and limitations, Supercritical Chromatography.

Imaging Techniques – Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM)

Hyphenated Techniques: HPLC-MS, GC-MS, GC-IR, ICP-MS and TLC-MS

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. J.H. Kennedy, Analytical Chemistry: Principles, 2nd ed. Saunders Holt, London, 1990
4. G. D. Christian; Analytical Chemistry, 5th ed. John Wiley & Sons, New York, 1994

5. 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
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 (CHH 505B)
Course Type	Core
Course Nature L-T-P-O Structure	Hard 0-0-12-0
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 $MgSO_4$ solution using M/100 EDTA in complexometric titration usingEriochrome Black T indicator titrimetrically
5. To estimate amount of calcium in standard CaCO3 solution using M/10 EDTA in complexometric titration usingEriochrome 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 aluminiumsulphate.
8. To estimate Ni2+ gravimetrically as Nickeldimethyl 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, PragatiPrakashan, 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, PragatiPrakashan, 2012
4. A. Gaddamwar and P. R. Rajput, Organic and Inorganic Practical Chemistry, PragatiPrakashan, 2010
5. J. Singh and L. D. S. Yadav; Advanced Practical Chemistry, Pragati Prakashan, 2012

SEMESTER II

Course Title/Code	Physical Chemistry-II (CHH 506B)
Course Type	Core
Course Nature L-T-P-O Structure	Hard 4-0-0-0
Objectives	To familiarize with concept of Quantum Chemistry in statistical thermodynaimics 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

Statistical Mechanics: Fundamentals: Idea of microstates and macrostates, Concept of distributions-Binomial & multi-nomial distributions for non-degenerate and degenerate systems, Thermodynamic probability and most probable distribution, Canonical and other ensembles, Statistical mechanics for systems of independent particles and its importance in chemistry, Types of statistics: Boltzmann, Bose-Einstein and Fermi-Dirac statistics, Thermodynamic probability
(W) for the three types of statistics, Derivation of distribution laws (most probable distribution) for the three types of statistics, Lagrange's undetermined multipliers, Stirling's approximation, Molecular partition function and its importance, Assembly partition function

SECTION-B

Thermodynamics Applications to ideal gases*:* The molecular partition function and its factorization, Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases, The electronic and nuclear partition functions, Calculation of thermodynamic properties of ideal gases in terms of partition function, Statistical definition of entropy, Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number, Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures.

SECTION-C

Diffraction Methods: Atomic scattering factors, Scattering by a small crystal, Direct and reciprocal lattice, Miller indices, Bragg's law and Laue's equations, Structure factor, Sy,tematic absences for different types of unit cells (primitive, face-centred, body-centred, side-centred) and application to some common metal and metal salt structures (rock salt, zinc blende). Space groups, Glide planes and screw axes, Structure determination for organic crystals like naphthalene, Fourier series **Patterson's functions** Heavy atom method, Comparison of X-ray method with electron and neutron diffraction methods,

SECTION-D

Kinetics: *Theories of reaction rates:* Collision theory, Potential energy surfaces (basic idea), Transition state theory (both thermodynamic and statistical mechanics formulations), Theory of

unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment)

Solution kinetics: Factors affecting reaction rates in solution, Effect of solvent and ionic Strength (primary salt effect) on the rate constant, Secondary salt effects

Books Recommended

1. McQuarrie, D. A. *Statistical Mechanics* Viva Books Pvt. Ltd.: New Delhi (2003).
2. Bagchi B. Statistical Mechanics for Chemistry and Material Science, CRC Press (2018).
3. L. D. Landau and E. M. Lifshitz, Statistical Mechanics, Part I, Butterworth-Heinemann, 3rd ed. (2005).
4. Kakkar, R., *Atomic & Molecular Spectroscopy* Cambridge University Press (2015).
5. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
6. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).

Course Title/Code	**Inorganic Chemistry-II (CHH 507B)**
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-I: Mechanisms of substitution reactions of tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral complexes; Potential energy diagrams, transition states and intermediates, Substitution reactions in octahedral complexes their mechanisms and kinetics, concept of lability and inertness on the basis of VBT and CFT, rate laws (Eigen-Wilkins mechanism, Fuoss Eigen equation), Acid hydrolysis, Base hydrolysis.

SECTION-B

Kinetics And Mechanism Of Substitution Reactions-II: Substitution in Square Planar Complexes, kinetics, Berry pseudorotation, Trans Effect and its applications to synthesis of complexes, theories of trans effect, mechanism, factors affecting rate of substitution, applications of complexes.

Metal complex sensitizers: Electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO_2 reduction.

SECTION-C

Electron Transfer Reactions-I : Mechanism and rate laws; various types of electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reductant, chemical activation. Precursor complex formation and rearrangement, Marcus-Husch theory, Nature of bridge ligands, fission of successor complexes, Two-electron transfers,Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes andinternal electron transfer.

SECTION-D

Electron Transfer Reactions-II: Redox reactions of metal complexes in excited states, correlation between thermal and optical electron transfer reactions; excited electron transfer reactions using $[Ru(bpy)_3]^{2+}$ complex and $[Fe(bpy)_3]^{3+}$ complex as examples. Role of spin-orbit coupling, life-times of excited states in these complexes

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, 3rded. ELBS, London, 1999
3. F. A. Cotton and G. Wilkinson;Advanced Inorganic Chemistry, 6thed.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 (CHH 508B)
Course Type	Core
Course Nature L-T-P-O Structure	Hard 4-0-0-0
Objectives	To familiarize carbon carbon multiple bond, ,aromaticity linear free energy relationship and advance heterocyclic reactions To impart knowledge on Elimination reactions
Outcome	Able to understant carbon carbon multiple bond, ,aromaticity linear free energy relationship and advance heterocyclic reactions Able to understand about Elimination reactions and its implication in organic chemistry
Prerequisites	Organic Chemistry-I

SECTION A

Addition To Carbon–Carbon Multiple Bonds: Electrophilic, free-radical and nucleophilic addition: Mechanistic and Stereo chemical aspects involving electrophiles, nucleophiles and free radicals, regio– and chemoselectivity, Orientation and reactivity. Hydrogenation of doubleand triple bonds, hydrogenation of aromatic rings.Hydroboration and Michael reaction, SharplessEpoxidation.

SECTION B

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

SECTION C

Nature of Bonding in Organic molecules: Delocalized chemical bonding –conjugation, cross conjugation, resonance, hyperconjugation, tautomerism. Aromaticity in benzenoid and nonbenzenoid compounds, alternante and non-alternante hydrocarbons, Huckel's rule

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 D

Heterocyclics With Two Hetero Atoms: Synthesis, reactivity, aromatic character and importance of the following heterocycles:Indole,Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine.Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole**.**

Books recommended

1. M.B. Smith and Jerry March; March's Advanced Organic Chemistry, 5th ed. John Wiley & Sons, New York, 2001
1. P. Sykes;A Guide Book to Mechanism in Organic Chemistry, 6th ed. Orient Longman Ltd., New Delhi, 1997
2. S. M. Mukherjee and S.P. Singh; Reaction Mechanism in Organic Chemistry, 1sted. Macmillan India Ltd., New Delhi, 1990
3. T.H. Lowry and K. S. Richardson; Mechanism and Theory in Organic Chemistry, 3rded. Addison – Wesley Longman Inc., 1998
4. P. S. Kalsi; Organic Reactions and Their Mechanisms, 1sted. New Age International Pub., New Delhi, 1996

Course Title/Code	**MOLECULAR SPECTROSCOPY (CHH 509B)**
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	Analytical Chemistry

SECTION A

Spectroscopy-I: Principle, Instrumentation and application of UV-visible, Molecular luminescence (fluorescence, chemiluminescence, phosphorescence)

Vibrational Spectroscopy: IR spectroscopy (Far IR and near IR), Raman Spectroscopy, Difference between Raman and IR spectra, Emission spectra

SECTION B

Spectroscopy-II: 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 C

Spectroscopy-III: 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 D

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

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 (CHH-510-B)
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	Laboratory work-I

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, PragatiPrakashan, 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, PragatiPrakashan, 2012

Course Title/ Code	**Scientific Research-1 (CHN-511-B)**
Course Type	Core
Course Nature	soft course
L-T-P-O Structure	0-0-0-4
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,1st ed. 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 andM. M. Jo Ray; Writing the Research Paper,1st ed. 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

(Physical Specialization)

Course title/code	SYMMETRY & GROUP THEORY (CHH 601B) [Common for all specialization]
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	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	Inorganic 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	Physical Special I: Magneto-chemistry, Chemical Kinetics, Catalysis & ion transport (CHH-602-B)
Course Type	Domain Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge of magnetochemistry To impart advanced knowledge and application of kinetics and electrochemistry
Outcome	Student will be able to 1. understand the knowledge of magnetochemistry and its application 2. understand knowledge and applications of kinetics and electrochemistry
Prerequisites	Physical Chemistry-I & II

SECTION-A

Magnetochemistry: Magnetic susceptibility and its determination, susceptibility equivalents, Pascal's law and its applications, Diamagnetism of elements, Compounds and its ions, Langevin's theory of paramagnetism, Curie's law, Weiss molecular field theory of paramagnetism, Curie- Weiss law, Determination of Curie point.

SECTION-B

Chemical Kinetics: Kinetics of fast reactions: Techniques of study of fast reactions with reference to stop flow, T-Jump, Flash photolysis and relaxation phenomena. Kinetics of oscillating reactions with special reference to Belousov-Zhabotinskii mechanism (B-Z mechanism)

SECTION-C

Catalysis & Kinetics: a) Oxidation of sugars by $K_3Fe(CN)_6$ and Cu^{+2} in alkaline medium, (b)Uncatalyzed and platinuem group metals (Osunium, ruthenium, iridium, palladium, rhodium etc.) Catalyzed oxidation of organic and inorganic compounds by $K_3Fe(CN)_6$ and Ce (IV) etc in acidic / alkaline medium.

SECTION-D

Ion Transport in solutions: Ionic movement under the influence of an electric field , mobility of ions, ionic drift velocity and its relation with current density, Einstein relation between the absolute mobility and diffusion coefficient, the Stokes- Einstein relation , the Nernst -Einstein equation, Waldens rule, the Rate- Process approach to ionic migration , the Rate process equation for equivalent conductivity, total driving force for ionic transport, Nernst - Planck Flux equation, ionic drift and diffusion potential , the Onsager phenomenological equations, The basic equation for the diffusion, Planck- Henderson equation for the diffusion potential

Reference Books

1. Peter Atkins & Julio De Paula, Physical Chemistry 10th Ed., Oxford University Press (2014).
2. G. W. Castellan, Physical Chemistry, 4th Ed., Narosa (2004).
3. G. A. McQuarrie, J. D. Simon, J. D., Molecular Thermodynamics, Viva Books Pvt. Ltd.: New Delhi (2004).
4. T. Engel, P. Reid, Physical Chemistry 3rd Ed., Prentice-Hall (2012).

5. M. J. Assael, A. R. H. Goodwin, M. Stamatoudis, W. A. Wakeham, S. Will, Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
6. S. S. Zundhal, Chemistry concepts and applications Cengage India (2011).
7. D. W. Ball, Physical Chemistry Cengage India (2012).
8. R. G. Mortimer, Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
9. I. N. Levine, Physical Chemistry 6th Ed., Tata McGraw-Hill (2011).
10. C. R. Metz, Physical Chemistry 2nd Ed., Tata McGraw-Hill (2009).

Course title/code	**Physical Special II** **Irreversible thermodynamics, Transport Phenomenon, Photochemistry & Fast Reaction (CHH 603B)**
Course Type	Domain Elective
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge of Irreversible thermodynamics, To impart advanced knowledge of transport phenomenon To impart photochemistry & Fast reactions
Outcome	Student will be able to 1. understand the knowledge of Irreversible thermodynamics, 2. understand knowledge of transport phenomenon 3. understand knowledge of photochemistry & Fast reactions
Prerequisites	Physical Chemistry-I & II

SECTION-A

Irreversible thermodynamics Meaning and scope of irreversible thermodynamics, Thermodynamic criteria for nonequilibrium states, Phenomenological laws- Linear laws, Gibbs equation, Onsager's reciprocal relations, Entropy production- specific examples of entropy production, Non-equilibrium stationary states, Prigogine's principle of maximum entropy production, Coupled phenomena. Some important applications of activation

SECTION-B

Transport phenomena: Diffusion coefficients, Fick's first and second laws, relation between flux and viscosity, relation between diffusion coefficient and mean free path, relation between thermal conductivity/viscosity and mean free path of a perfect gas, Einstein relation, Nernst-Einstein equation, Stokes-Einstein equation, Einstein-Smoluchowski equation.

SECTION-C

Photochemistry: Primary and secondary processes in photochemistry, Fate and properties of excited states, Photolumineseence and Photostationary state, Photosensitization, Rice – Herzfeld mechanisms. Photochemical chain reactions (hyderogen and chlorine, hydrogen and bromine) Non-chain photochemical reactions (formation of phosgene, decomposition of H_2O_2 in presence of CO)

SECTION-D

Fast reactions: Luminescence and energy transfer processes, study of kinetics by stopped-flow technique, relaxation method, flash photolysis and magnetic resonance method, Kinetics of solid-state reactions size of a hole

Reference Books

1. Katchalsky, A. & Curren, P. F. *Non Equilibrium Thermodynamics in Biophysics* Harvard University Press: Cambridge (1965).
2. Kalidas, C. & Sangaranarayanan, M.V. Non-Equilibrium Thermodynamics: Principles & Applications, Macmillan India Ltd. (2002).
3. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).
4. Thomas, J. M. & Thomas, M. J. *Principles and Practice of Heterogeneous Catalysis* John Wiley & Sons (1996).
5. Chorkendorff, Ib. & Niemantsverdriet, J. W. *Concepts of Modern Catalysis and Kinetics* Wiley-VCH (2003).
6. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).

Course title/code	**Physical Elective-I Advanced Spectroscopy (CHH 604 B)**
Course Type	Domain Elective
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge of qualitative treatment of spectroscopic To impart advanced knowledge and application of kinetics and electrochemistry
Outcome	Student will be able to 1. understand the knowledge of magnetochemistry and its application 2. understand knowledge and applications of kinetics and electrochemistry
Prerequisites	Physical Chemistry-I & II

SECTION-A

Molecular Structure and Spectroscopy Spectroscopic methods*:* Characterization of electromagnetic radiation, Born- Oppenheimer approximation, Heisenberg's Uncertainty Principle, Basic elements of spectroscopy, Time dependent perturbation, Einstein coefficients, Lambert-Beer's law, Integrated absorption coefficients, Transition dipole moments and general selection rules based on symmetry ideas

Atomic spectra: Characterization of atomic states, Microstate and spin factoring methods, Hund's rules, Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials), Spectra of complex atoms, Zeeman and Stark effects, Atomic photoelectron spectroscopy,

SECTION-B

Introduction to rotational spectroscopy: Rotational spectroscopy of diatomic molecules based on rigid rotator approximation, Determination of bond lengths and/ or atomic masses from microwave data, Effect of isotopic substitution, Non-rigid rotator, Classification of polyatomic molecules, Energy

levels and spectra of symmetric top molecules and asymmetric top molecules, First order Stark effect

Vibrational spectroscopy: Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules, Extension to polyatomic linear molecules, Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation, Force constants and amplitudes. Anharmonic oscillator, Overtones and combination bands

SECTION-C

Electronic spectroscopy: Diatomic molecules, Selection rules, Breakdown of selection rules, Franck-Condon factors, Dissociation energies, Photoelectron spectroscopy of diatomic (N2) and simple polyatomic molecules (H2O, formaldehyde), Adiabatic and vertical ionization energies, Koopmans' theorem, Polyatomic molecules, Oscillator strengths, Use of Free Electron Model, HMO theory and Group theory for polyenes and carbonyl compounds (formaldehyde), Qualitativeideas of solvent effects- viscosity, polarity, hydrogen bonding

Excited states: Deactivation, Jablonskii diagram, Fluorescence and phosphorescence and factors affecting these calculations of excited state life-times from absorption data, Quenching of fluorescence, Stern-Volmer equation

SECTION-D

NMR spectroscopy: Larmor precession, Mechanisms of spin-spin and spin-lattice relaxations and quantitative treatment of relaxation, Quantum mechanical treatment of the AB system, Selection rules and relative intensities of lines

Principles of Mossbauer spectroscopy: Isomer shifts, Quadrupole and Nuclear Zeeman splittings, Applications in structure determination

Reference Books

1. Hollas. J. M. *Modern Spectroscopy* 4th Ed., John Wiley & Sons (2004).
2. Barrow, G. M. *Introduction to Molecular Spectroscopy* McGraw-Hill (1962).
3. Kakkar, R., *Atomic & Molecular Spectroscopy* Cambridge University Press (2015).
4. Brand, J. C. D. & Speakman, J. C. *Molecular Structure: The Physical Approach* 2nd Ed., Edward Arnold: London (1975).
5. Chang, R. *Basic Principles of Spectroscopy* McGraw-Hill, New York, N.Y. (1970).
6. Moore, W. J. *Physical Chemistry* 4th Ed. Prentice-Hall (1972).
7. Warren, B. E. *X-Ray Diffraction* Dover Publications (1990).
8. Bacon, G. E. *Fifty Years of Neutron Diffraction* Hilger (1987).

Course title/code	**Physical Elective-II** **Advanced Chemical Kinetics (CHH 605 B)**
Course Type	Domain Elective
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart knowledge advanced chemical kinetics
Outcome	Student will be able to understand the knowledge of advanced chemical kinetics
Prerequisites	Physical Chemistry-I & II

SECTION-A

Statistical theories of kinetics: Collision theory, Activated Complex theory, Potential energy surfaces- attractive and repulsive forces, Lindemann's theory of unimolecular reactionsenergy transfer, fall-off region and its limitations, Rice-Ramsperger and Kassel (RRK) model, and Marcus refinement of RRK model (RRKM) for the calculation of rate constants of simple unimolecular (isomerization) reactions.

SECTION-B

Enzyme kinetics: Michaelis-Menten mechanism - single and double intermediates, King- Altman method for working out the kinetics of complex enzyme reactions

Enzyme inhibition- reversibility and products inhibition, Computer simulation in chemical kinetics

SECTION-C

Reaction Dynamics I: Molecular beams, principle of crossed-molecular beams, Molecular encounters and principal parameters, e.g. Impact parameter, Collision cross-section, Reaction cross-section and relation between reaction cross-section and reaction rate (single velocity), Dependence of collisional cross-section on translational energy

SECTION-D

Reaction Dynamics II: Probing the transition state, Dynamics of barrier less chemical kinetics in solution, dynamics of unimolecular reactions and bimolecular reactions

Reference Books

1.Pilling, M. J. & Seakins, P. W. *Reaction Kinetics* Oxford Press (1997).
2. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997). .

Course title/code	**Physical Laboratory (CHH 606B)**
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	0-0-8-0
Objectives	To make student able to understand the practical aspects of kinetics of the reactions & different potentiometric titrations
Outcome	Student will be able to the exposure of practical aspects of kinetics of the reactions & different potentiometric titrations. Student will be able to understand the research and experimental outcome analysis.
Prerequisites	Laboratory work-II

List of Experiments

1. Determine the concentration or percentage of one or two optically activesubstances in the given solution polarimetrically.
2. Kinetics of oxidation of reducing sugars by potassium ferricyanide/ copper(II) in presence of ammonium hydroxide or sodium hydroxide.

3. Kinetics of oxidation of alcohols/diols by aqueous alkaline hexacyanoferrate (III) ions.
4. Potentiometric titration of weak/strong acid and strong /weak base.
5. Study of the oxidation of cyclic alcohols by cerium(IV) sulphate in acidic medium in presence of Iriduum(III) chloride.
6. Kinetics of iridium (III) catalyzed oxidation of aromatic aldehydes/aromatic alcohols/hydrocarbons by cerium (IV) in aqueous acidic medium.
7. Kinetics of Ru(III) catalysed oxidation of alcohols/diols by Ce(IV) sulphate in acidic medium .
8. Kinetics of oxidation of aliphatic/cyclic alcohols/glycols by alkaline hexacyanoferrate(III) catalyzed by ruthenium (III) chloride

Course Title/ Code	**Scientific Research-II (CHN 607B) (COMMON FOR ALL SPECIALIZATIONS)**
Course Type	Core
Course Nature	soft course
L-T-P-O Structure	0-0-0-4
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

SEMESTER III

(Inorganic Chemistry Specialization)

Course title/code	**Inorganic Special-I** **Organometallic Chemistry of Transition Metals & Bio Inorganic Chemistry (CHH 608B)**
Course Type	Domain Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To conceptualize the concept of bonding between organic ligands and transition metals. To Understand physical and chemical properties of various classes of organometallic compounds. To understand role of metal ions on biological system. To apply the knowledge of metal toxicity in development of chelating agents for metal detoxification.
Outcome	The student will be able to extent applications of organometallic compounds in catalysis, and other industrial processes. The student will be able to understand the use of Transition Metal Compounds in biological system.
Prerequisites	Inorganic Chemistry-I & II

SECTION A

Organometallic compounds-I: Introduction, Stable electron configurations, Electron count preference, Electron counting and oxidation states, Nomenclature.

Ligands: Carbon monoxide, Phosphines, Hydrides and dihydrogen complexes, Alkyl, alkenyl, alkynyl, and -aryl ligands, Alkene and alkyne ligands, Nonconjugated diene and polyene ligands. Butadiene, cyclobutadiene and cyclooctatetraene, Benzene and other arenes, The allyl ligand, Cyclopentadiene and cycloheptatriene, Carbenes, Alkanes, agostichydrogens, and noble gases, Dinitrogen and nitrogen monoxide

SECTION B

Organometallic compounds-II: d-Block carbonyls (Preparation, Properties), Metallocenes, Metal - Metal bonding and metal clusters. Reactions: Ligand substitution, Oxidative addition and reductive elimination, σ -Bond metathesis, 1,1-Migratory insertion reactions, 1,2-Insertions and β –hydride Elimination, Nucleophilic and Electrophilic attack, Hydride eliminations and cyclometallations

SECTION C

Bio-Inorganic Chemistry-I: Fundamentals of inorganic biochemistry, geo-chemical effects on life systems, essential and non-essential elements in bio-systems.Role of alkali/alkaline earth metals in bio-systems, Role of 3*d* block elements and nonmetalsin bio-systems, Role of metal ions in oxygen carriers and synthetic oxygen carriers.Designing of chelating agents and metal chelates as medicines, Fixation of dinitrogenbiologically and abiologically, biotransformation of nonmetallic inorganic compounds, Environmental bioinorganic chemistry, Metal ions as probes for locating active sites, Biocatalysts

SECTION D

Bio-Inorganic Chemistry-II: Inhibitions as competitive and non-competitive, metals and metalloproteins, Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA),

Templatetemperature, stability of DNA, Role of metal ions in replication and transcription process of nucleic acids, Biochemistry of di oxygen, bioinorganic chips and biosensors, Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, calcification reclaiming of barren land. Cytochromes, ferrodoxins and iornsulphur proteins, ion transport across membranes, Biological nitrogen fixation, PSI, PS – II, Oxygen uptake proteins

Reference Books

1. Bioinorganic Chemistry Williams, An Introduction to Bioinorganic Chemistry
2. M. N. Hughes, Inorganic Chemistry of Biological Processes
3. Ochiai: Bioinorganic Chemistry: Allyn& Bacon Burton
4. P. L. Pauson, Organometallic Chemistry
5. T. S. Swain and D. S. T. Black, organometallic Chemistry
6. Eichhorn: Inorganic Biochemistry : Vol I , 2 Elsevier
7. Williams: an Introduction to Bioinorganic Chemistry, C.C. Thomos Spring III
8. Wallace: Decade on synthetic chelating agent in Inorganic plant nutrition, Wallace

Course title/code	**Inorganic Special-II: Supramolecular Chemistry & Metal Clusters (CHH 609B)**
Course Type	Domain Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To conceptualize the concept of supramolecular interactions,macrocyclic compounds and template synthesis To Understand chemical properties of cages, metal clusters, carboranes, phosphazies. To understand role of silicates and aluminosilicates To conceptualize the concept of clays, zeolites and its applications
Outcome	The student will be able to extent applications of supramolecular molecules and other industrial process The student will be able the understand the use of zeolites, clays, silicates, aluminosilicates in industrial appliatications.
Prerequisites	Inorganic Chemistry-I & II

SECTION A

Supramolecular Chemistry-I: Molecules and Supramolecules, Supermolecules, Large Molecules Classification,Nomenclature, Thermodynamic and Kinetic selectivity, Supramolecular interactions, Supramolecularhost design, Macrocyclic versus acyclic hosts, Chelate Macrocyclic and macrobicyclic hosts, Highdilution synthesis, Template synthesis

SECTION-B

Supramolecular Chemistry-II: Molecular recognition: Receptors, design and synthesis of co-receptors and multiple recognition, Hydrogen bonds, strong, weak and very weak H-bonds,

Utilisation of H-bonds to create supramolecular structures, Use of H-bonds in crystal engineering and molecular recognition, Chelate and macrocyclic effects.

SECTION C

Chemistry of Inorganic Rings, Cages and Metal Cluster Compounds-I: Chemistry of inorganic rings, cages and metal cluster compounds, borazines, phosphazenes, polyhedral boranes, carboranes, metalloboranes and metallocarboranes

Silicates and aluminosilicates: Classifications, structure, properties and applications of naturally occurring silicates andaluminosilicates.

SECTION D

Chemistry of Inorganic Rings, Cages and Metal Cluster Compounds-II: Syntheses 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 catalyses

Reference Books

1. Ballhausen C. J. *Introduction to Ligand Field Theory* McGraw Hill Book Co.: N.Y (1962).
2. Marshal, C. E. *The Physical Chemistry and Minerology of Soil Vol. I Soil Materials* John Wiley & Sons.
3. Wells, A. F. *Structural Inorganic Chemistry* Oxford University Press.
4. Adams, D. M. *Inorganic Solids. An Introduction to Concepts in Solid-State Structural*
1. *Chemistry* John Wiley & Sons
5. Azaroff, L. V. *Introduction to Solids* Tata McGraw Hill Publishing Co. Ltd.
6. Breck, D. W. *Zeolites Molecular Sieves- Structure, Chemistry and Use.* John Wiley & Sons.

Course title/code	**Inorganic Special-Elective: Solid state Materials (CHH 610B)**
Course Type	Domain Elective
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To familiarize students with the concept of solids, their properties, preparation methods, etc. To gain the knowledge of the chemistry between layered structures of solids
Outcome	Students will be able to understand the structural aspects of inorganic solid substance and properties associated with different solid structures.
Prerequisites	Inorganic Chemistry I and II

Section A

Electronic, Electric and Optical behaviour of Inorganic materials: Electronic structure of solids, band theory, band structure of metals, insulators and semiconductors, the band gap, Intrinsic and extrinsic semiconductors, doping of semiconductors and conduction mechanism, temperature dependence of conductivity, carrier density and carrier mobility in semiconductors, synthesis and purification of semiconducting materials, single crystal growth, rectifier transistors, optical devices

Section B

Methods to synthesize solid-state materials: Ceramic method, solid-state reaction and its kinetics, hydrothermal, sol-gel, co-precipitation (precursor), vapor phase transport methods.

Amorphous inorganic materials: Glasses, refractories, materials obtained from organometallic chemical vapor deposition (MOCVD)

Section C

Inorganic Polymers: Classification, types of Inorganic polymers, Chemistry of following polymers a) Silicones b) phosphonitric halides c) condensed phosphates d) coordinated polymers e) Silicates f) Isopoly & heteropoly acids

Solid State lasers (Ruby, YAG and tunable lasers): Inorganic Phosphor materials, synthesis and advantages of optical fibers, over conducting fibers

Section D

Mesoporous materials and their catalytic applications: Various types of mesoporous materials (oxides, sulphides), tailoring of pore size, applications of mesoporous materials in heterogeneous catalysis

Intercalation chemistry: Introduction, intercalation reactions in graphite, layered double hydroxides, layered sulfides, applications of intercalation chemistry

Course title/code	**Inorganic Elective: Inorganic and Biological Catalysis (CHH 611B)**
Course Type	Domain Elective
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To conceptualize the concept of catalyst and their importance in industrial applications To understand the concept of toxicology an detoxification in biological systems.
Outcome	The student will be able to extent applications of inorganic catalyst in various industries The student will be able to understand the use of inorganic and biological catalyst in various biochemical reactions.
Prerequisites	Inorganic I & II

SECTION A

Catalysis I: ligands in homogeneous catalysis such as CO, amines, phosphines, NHC's, alkenes, alkynes, carbenes, carbynes, etc.General principles, Homogenous Catalysis (alkene metathesis,Types of metathesis such as RCM, ROM, ROMP, ADMET and EM

hydrogenation of alkenes, hydroformylation, Wacker oxidation on alkenes, asymmetric oxidation, methanol carbonylation.

SECTION B

Catalysis II: Heterogenous catalysis (nature of heterogenous catalysts, hydrogenation catalysts, catalytic cracking), electrocatalysis, Hybrid Catalysis. Grubbs I, II and III, Schrock and Schrock-Hoveyda catalysts, Fischer Tropsch process, C-H activation of alkyls and aryls uing transition metal complexes.

SECTION C

Catalysis III: Applications in Industry: Palladium and Nickel catalyzed cross coupling reactions such as Suzuki, Heck, Sonogashira, Stille Coupling, Negishi, Hiyama coupling, Buchwald-Hartwig, decarboxylative cross coupling and alpha arylation of carbonyls.

SECTION-D

Toxicology: Metal poisoning and treatment by using chelating agent, mercury, lead & cadmium poisoning & treatment. Metals in the regulation of biochemical events, Transport and storage of metal ions in vivo. Biochemistry of calcium as hormonal messenger, and neurotransmitter. Fundamentals of toxicity and detoxification.

Reference Books

1. Principles of Bioinorganic chemistry, S .J. Lippard and J. M. berg
2. Bioinorganic chemistry, I. bertini, H. B. Gray, S. J. Lippard, and J. S. Valentine
3. Progress in inorganic chemistry Vol.I and Vol.II .ed. G. L. Eichom, Elsevier
4. Progress in inorganic chemistry Vols 18 and 38 ed. J. J. Lipard, Wiley.

Course title/code	Inorganic Laboratory (CHH 612B)
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	0-0-8-0
Objectives	To impart the laboratory exposure to the synthesis of coordination complexes and quantitative analysis of the inorganic mixtures
Outcome	Students will be able to hands on laboratory exposure to the synthesis of coordination complexes and quantitative analysis of the inorganic mixtures
Prerequisites	Physical Chemistry-I & II

List of Experiments

1. Quantitative separations and determinations of following pairs of metal ions using gravimetric and volumetric methods
   (a) Ag^{+}/Cu^{2+} (b) Cu^{2+}/Zn^{2+} (c) Fe^{3+}/Ca^{2+} (d) Ba^{2+}/Cu^{2+}
   (e) Ni^{2+}/Zn^{2+} (f) Ag^{+}/Ni^{2+} (g) Fe^{3+}/Ni^{2+}
2. Inorganic Preparations of the following compounds
   (a) Prussian Blue (b) Trisacetylacetonato Iron (III)
   (c) Tetraammine copper (II) sulphate monohydrate
   (d) Hexamine cobalt (III) hexanitritocobaltate (III)
   (e) Sodium hexanitritocobaltate (III)

Reference 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. PragatiPrakashan, 2010
2. A. I. Vogel; Vogel's textbook of Practical Inorganic Analysis, 5th ed. Longman Scientific and technical Publisher, UK, 1989

SEMESTER III

(Organic Specialization)

Course title/code	Organic Special-I: Statistical Stereochemistry & Asymmetric Synthesis (CHH 613B)
Course Type	Core
Course Nature	Hard
L-T-P-O Structure	4-0-0-0
Objectives	To impart the knowledge of stereochemistry of the organic molecules. To impart the knowledge of various methods of asymmetric synthesis
Outcome	Student will be able to 1. Understand the nomenclature, configuration and stereochemistry of cyclic and acyclic molecules. 2. Understand the various methods of to induce asymmetry in the molecules.
Prerequisites	Organic Chemistry-I & II

SECTION A

Stereochemistry-I: Configurational Isomerism (optical and geometrical), Resolvable and non-resolvable compounds, Geometrical isomerism (single bond, multiple bond and monocyclic, bicyclic, bridging and polycyclic structure), and threo-erythro nomenclature, representation and interconversion of Fischer, Newman, Sawhorse and flying wedge formulae, Relative and absolute configuration, Epimers and anomers

SECTION B

Stereochemistry-II: Relationship between the molecules: homologues, conformational, configurational, epimers, anomers, geometrical, optical, enentiomers, identical, diastereomers etc. Axis of chirality and plane of chirality (ANSA compounds, p-cyclophanes, transcyclooctene), optical isomerism in allenes, biphenyls (atropoisomerism), bipyrolles, binapthols, spiranes, hemispiranes.elementary ideas about stereochemistry of tertiary amines, quaternary salts, sulphur and phosphorous compounds.

SECTION C

Stereochemistry-III: Topicity of ligands, lone pairs and faces, their nomenclature and prochiralcentre. Stereospecific and stereoselective reaction.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. Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio.

SECTION D

Methodologies in Asymmetric Synthesis: Strategies in Asymmetric Synthesis:

I.Chiral substrate controlled: Nucleophilic additions to chiral carbonyl compounds (Cram's rule), α-alkylation through oxazolines and azaenolates, α-alkylation using imines, Ender's asymmetric α-alkylation of hydrazones of aldehydesand ketones,

2.Chiral auxiliary controlled: 1, 4 Asymmetric induction (Prelog's rule), α-alkylation of amino acids via imidazolidinones, α-alkylation ofrα-hydroxyl acids via lactones, asymmetric α-alkylation of glycine, evans alkylation of S-prolinol

3.Chiral reagent controlled: enantioselective hydroboration i.e. use of chiral boronhydrides(hydroborations with diispinocampheylborane and hydroborations with monoispinocampheylborane) and Chiral trialkylboranes(Midland's reagent)

4.Chiral catalyst controlled: Jacobsen epoxidation, homogenous hydrogenation, ChiralRu and Rh catalysts for homogenous asymmetric hydrogenation.

Reference Books

1. Jonathan Clayden, Nick Geeves, Stuart Warren, Organic Chemistry, Oxford University Press, second edition
2. D. Nasipuri, Stereochemistry of Organic Compounds-Principles & Applications, New Age International.
3. P.S. Kalsi, Stereochemistry of Organic Compounds- Conformation and Mechanism: New Age International.
4. Ernest L Eliel& Samuel H. wilen, Stereochemistry of Carbon compounds.
5. R S Ward, Stereo selectivity in organic synthesis
6. Howard, S. I.; Morrison, J. D. Asymmetric Synthesis; Academic: New York. 1983; Vol. 2.
7. Nogradi. M. Stereoselective Synthesis.

Course title/code	**Organic Special-II: Photochemistry And Pericylic Reaction (CHH 614B)**
Course Type	Core
Course Nature	Domain
L-T-P-OStructure	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, photocycloadditions, photodimerisation of simple andconjugated 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.

Reference Books

1. J. Singh and J. Singh; Photochemistry and Pericyclic reactions, 3rded. 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	**Organic Special-Elective: Modern Organic Synthetic Technique (CHH 615B)**
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 Chemistry-I & II

SECTION A

Hybrid Transfer Reagents: Sodium borohydride**,** lithium aluminum hydride and alkoxy substituted LAH reducing agents, DIBAL,

Common Named Reactions And Rearrangements – applications in organic synthesis

Name Reaction: Appel, Birch, Cannizzaro, claisen, Clemmenson, Curtius, Dakin-West, Eschweiler-clarke, Finkelstein, Gabriel, Heck, Mannich, Negishi cross-coupling, Prins, Ritter, Stille, Suzuki, Sonogashira coupling, Swern, Ullman, Wittig Reactions

Rearrangement: Beckmann, Cutius, The Lossen, Baeyer-Villager, Favorskii, Fries, Claisen, Benzilic acid, Wagner Meerwin rearrangement, Pinacol-pinacolone rearrangements and Wolf Rearrangement

SECTION B

Redox Reactions: Oxidation - Introduction, Different oxidative processes for the followings:Hydrocarbons- al kenes, aromatic rings, saturated C-H groups (activated andunactivated). Alcohols, diols, aldehydes, ketones, and carboxylic acids

Reduction – Introduction, Different reductive processes for followings: Hydrocarbons – alkanes, alkenes, alkynes and aromatic rings. Carbonylcompounds – aldehydes, ketones, acids and their derivateives. Nitro compounds.

SECTION C

Newer Synthetic Reactions and Reagents: Enolates, enonate equivalents and **enamines**:Applications in carbon-carbon bond formation and related reactions.

Phosphorus*,* Sulphur and nitrogen ylides*:*** Preparation, applications in organic synthesis andmechanism.

Principles and applications of phase transfer catalysis, crown ethers and polymer-supportedreagents in organic synthesis.

SECTION D

Philosophy of organic synthesis: Disconnection approach, one group and two groupdisconnections, reversal of polarity, chemoselectivity, one group C-C disconnection, twogroup C-C disconnections, 1,3-difunctional and 1,5-difunctional compounds. **Umpolung reactions** (sulphur compounds, nitro compounds, lithiated ethers and relatedcompounds).

Reference Books

1. 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

Course title/code	**Organic Special-Elective: Bioorganic Chemistry (CHH 616B)**
Course Type	Core
Course Nature	Elective
L-T-P-OStructure	4-0-0-0
Objectives	To impart the knowledge of the activity of the organic biomolecules and its applications in biological systems
Outcome	Student will be able to understand the activity of the organic biomolecules and its applications in biological systems
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 & 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, Chiralhydroxy 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 uridinediphospho sugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

Reference Books:

Course title/code	**Organic Special-Elective: Chemistry of Natural Products (CHH 617B)**
Course Type	Core
Course Nature	Elective
L-T-P-OStructure	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	**Organic I & II**

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	**Organic Laboratory (CHH 618B)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-8-0
Objectives	To familiarize with synthesis of organic compounds To familiarize with separation 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 Vanadylacetyloacetonate

LIST OF EXPERIMENTS

TO SEPARATE AND ANALYSE THE ORGANIC COMPOUNDS

9. Mixture of benzoic acid and β-naphthol
10. Mixture of m-notroaniline and hydroquinone
11. Mixture of tetrahydrofuran and cinnamic acid
12. Mixture of chloroform and benzidine
13. Mixture of aniline and benzamide
14. To prepare Chalcone (Benzene acetophenone)
15. To extract caffeine from tea leaves
16. To extract piperine from Black pepper
17. To prepare Dichlorodipyridinocobalt (II)
18. To prepare ammonium diamminetetrathiocyanato chromate (III)

Reference 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. PragatiPrakashan, 2010
2. A. I. Vogel; Vogel's textbook of Practical Organic Chemistry, 5th ed. Longman Scientific and technical Publisher, UK, 1989
3. H. L. FieserandF. L. Fieser, Organic Chemistry, Vol 1-11, Trade ed. 1944
4. B. M. Trost, I. fleming and S. L. Scheiber; Comprehensive Organic Synthesis, 1st ed. Pergamon Press, 2007

SEMESTER IV

(FOR ALL SPECIALIZATIONS)

Course Title/Code	**Major Project (CHN 619 B)**
Course Type	Core
Course Nature **L-T-P-O Structure**	Hard 0-0-0-12
Objectives	To impart understanding of research papers/articles in specific areas To improve the communication skills by presentation on specific subjects To improve the team work To improve the research and practical approach
Outcome	Student will be able to Understand research and innovation skills Enhance their communication skills Start working in a team and improve their problem solving skills