ST. JOSEPH’S UNIVERSITY

BENGALURU - 27

SCHOOL OF CHEMICAL SCIENCES

DEPARTMENT OF CHEMISTRY

SYLLABUS FOR POSTGRADUATE COURSE
M.Sc. ORGANIC CHEMISTRY

2022-2024

Re-accredited with ‘A++’ GRADE and 3.79/4 CGPA by NAAC
Recognised as “College of Excellence” by UGC

FROM 2022 ONWARDS

Department of Chemistry

The Postgraduate programme in chemistry is designed to give students a good foundation in Chemistry and develop in them problem solving and experimental skills so that they are well prepared for further studies in specialized areas of Chemistry or for employment in academic institutions and in industry.

Mission statement:

- To promote among our learners the skills of thinking, experimentation and application of the knowledge gained.
- To promote concern for the environment and to develop appreciation for green Chemistry.
- To prepare our students for life in the larger community.

Benchmark Statements for the Course:

- To instill in students a sense of enthusiasm for chemistry, an appreciation of its application in different contexts, and to involve them in intellectually stimulating and satisfying experience of learning and studying.
- To provide students with a broad and balanced foundation of chemical knowledge and practical skills.

Teaching-Learning:

Although the lecture method is extensively used, the students are also encouraged to do self-study through other activities like assignments, seminars, quiz, viva-voce etc.

Co-curricular Activities:

The Chemical Society for P.G. students provides them with a platform to interact with students of other institutions and also with eminent scientists from universities, other academic institutions and industries.

Course Details: The course details for the P.G. programme are as follows:

SUMMARY OF CREDITS

SEMESTER	PAPER CODE AND TITLE	NO. OF TEACHING HOURS	NO. OF CREDITS	TOTAL MARKS
SEMESTER I				
THEORY				
Paper I	**CH7121:** Inorganic Chemistry - I	60	04	100
Paper II	**CH7221:** Organic Chemistry - I	60	04	100
Paper III	**CH7321:** Physical Chemistry - I	45	03	100
Paper IV	**CH7421:** Spectroscopy -I	60	04	100
Paper V	**CH7521:** Principles of Chemical Analysis	60	04	100
PRACTICAL				
Paper I	**$CH7P_1$** Inorganic Chemistry Practical I	44	1.5	50
Paper II	**$CH7P_2$** Inorganic Chemistry Practical II	44	1.5	50
Paper III	**$CH7P_3$** Organic Chemistry Practical I	44	1.5	50
Paper IV	**$CH7P_4$** Organic Chemistry Practical II	44	1.5	50
		TOTAL	**25**	**500**
SEMESTER II				
THEORY				
Paper I	**CH8121:** Inorganic Chemistry II	60	04	100
Paper II	**CH8221:** Organic Chemistry II	60	04	100
Paper III	**CH8321:** Physical Chemistry II	60	04	100
Paper IV	**CH8421:** Spectroscopy II	60	04	100
Paper V	**CH8521:** Separation Techniques	45	03	100

Note: Students can choose one of the departmental elective from Paper V-A or V-B				
PRACTICAL				
Paper I	**CH8P1** Physical Chemistry Practical I	44	1.5	50
Paper II	**$CH8P_2$** Physical Chemistry Practical II	44	1.5	50
Paper III	**$CH8P_3$** Preparation and characterization - I	44	1.5	50
Paper IV	**$CH8P_4$** Preparation and characterization - II	44	1.5	50
		TOTAL	**25**	**600**

SEMESTER	**PAPER CODE AND TITLE**	**NO. OF TEACHING HOURS PER WEEK**	**NO. OF CREDITS**	**TOTAL MARKS**
SEMESTER III				
THEORY				
Paper I	OCH9122: Organic Synthesis-I	4	4	60
Paper II	OCH9222: Organic Synthesis-II	3	3	60
Paper III	OCH9322: Chemistry of Heterocyclic Compounds, Biomolecules and Natural Products	4	4	60
Paper IV	OCH9422: Stereochemistry and asymmetric synthesis	4	4	60
Paper V (OE)	CHOE 9521: Open elective: Life's laboratories CHOE 9622: Culinary Chemistry	2	2	30
Note: Students choose open elective from other departments.				

PRACTICAL				
Paper I	OCH9P1: Separation and identification of organic compounds	4	1.5	50
Paper II	OCH9P2: Organic Synthesis - 1 (one-stage and two-stage preparations)	4	1.5	50
Paper III	OCH9P3: Organic Synthesis-II (advanced organic synthesis)	4	1.5	50
Paper IV	OCH9P4: Organic Synthesis-III (green methods of organic synthesis)	4	1.5	50
		TOTAL	**6**	**200**
SEMESTER IV				
Paper I	OCH0221: Medicinal Chemistry	4	4	60
Paper II	Dept Electives CHDE 0221: Chemistry of Materials CHDE 0321: Green Chemistry and Diversity of its Applications CHDE 0421: Forensic Chemistry CHDE 0521: Supramolecular Chemistry	4	4	60
	CH0PR PROJECT WORK	**42/week**	**14**	**100**
	IGNITORS/ OUTREACH		**04**	

Total No. of Credits : 26
KEY WORDS: DE – Departmental Elective and OE – Open Elective

Note: One credit is equivalent to one hour of teaching (lecture or tutorial) or three hours of practical work/field work per week.

CREDITS FOR M.Sc. CHEMISTRY						
I -II SEMESTER						
	T/P	**Number of Teaching hours per week**	**CREDITS**	**Total Teaching hours in a semester**	**TOTAL CREDITS IN ONE SEMESTER**	**TOTAL CREDITS IN ALL SEMESTERS**
Optional Subjects					25	25 x 2 = 50
A	T	4	4	60		
B	T	4	4	60		
C	T	4	4	60		
D	T	4	4	60		
E	T	3	3	45		
Practical-I	P	4.5	1.5	50		
Practical –II	P	4.5	1.5	50		
Practical-III	P	4.5	1.5	50		
Practical –IV	P	4.5	1.5	50		
III SEMESTER						
Optional Subjects					25	25
A	T	4	4	60		
B	T	4	4	60		
C	T	3	3	45		
Elective subject	T	4	4	60		
Open elective	T	2	2	30		
Practical-I	P	4.5	1.5	50		
Practical –II	P	4.5	1.5	50		
Practical-III	P	4.5	1.5	50		
Practical –IV	P	4.5	1.5	50		
Outreach Programme			2			
IV						

SEMESTER						
A	T	4	4	60	25	25
B	T	4	4	60		
PROJECT	P	42	15	100		
IGNITORS			2			
TOTAL						**100**

FIRST SEMESTER

THEORY PAPERS

Semester	I
Paper code	CH7121
Paper title	INORGANIC CHEMISTRY - I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. CHEMICAL BONDING **13 hrs**

(Recall: Lewis Structures: The octet rule, resonance, VSEPR theory). Valence Bond theory: homonuclear diatomic molecules (H_2 & N_2), polyatomic molecules (H_2O), hypervalence (PCl_5 and SF_6), hybridization. Molecular orbital theory: introduction to wave functions for molecular orbitals, LCAO approach, symmetry and overlap, symmetry of molecular orbitals, homonuclear diatomic molecules and molecular ions (H_2 to O_2), heteronuclear diatomic molecules (HF, CO, BeH_2 and ICl), bond order and magnetic property. Polyatomic molecules – molecular orbitals of NH_3, hypervalence in the context of molecular orbitals (SF_6), molecular shapes in terms of molecular orbitals - Walsh diagram (XH_2), structure and bond properties – bond length, bond strength, electronegativity and bond enthalpy, Pauling scale of electronegativity, Ketelaar triangle, Bent's rule, δ (delta) bond and agostic interactions.

2. THE STRUCTURES OF SIMPLE SOLIDS **15+2 hrs**

Unit cells and the description of crystal structures - the close packing of spheres, holes in close-packed structures. Structures of metals and alloys, polytypism, nonclose-packed structures, polymorphism of metals, atomic radii of metals, Goldschmidt correction. Alloys - substitutional solid solutions, interstitial solid solutions of nonmetals, intermetallic compounds, Zintl phases. Ionic solids-characteristic structures of ionic solids, binary phases AX_n: rock-salt, cesium-chloride, sphalerite, fluorite, anti-fluorite, zinc blende and wurtzite, nickel arsenide and rutile, ternary phases ABX_3, AB_2X_4 and $B(AB)X_4$: perovskite, spinel and inverse spinel structures. Rationalization of structures - ionic radii, radius ratio, structure maps. The energetics of ionic bonding, lattice enthalpy and Born–Haber cycle, calculation of lattice enthalpies, Born-Lande equation-derivation - comparison of experimental and theoretical values - Kapustinskii equation, consequences of lattice enthalpies.

Defects and nonstoichiometry - Intrinsic point defects - Schottky defect, Frenkel defect -

<u>Predicting defect types - Extrinsic point defects-F-centre, nonstoichiometric compounds</u>.

3. CHEMISTRY OF THE MAIN GROUP ELEMENTS 18 + 2hrs

Polymorphism of carbon, phosphorus and sulphur: Structure-property correlation in diamond and graphite, intercalation compounds of graphite, carbon nanotubes-types and preparation, structureof fullerene (C_{60}). Differences among white phosphorus, black phosphorous and red phosphorous with special emphasis on structural aspects. Cyclosulphur and polycatenasulphur. Boranes: Classification, preparation of higher boranes by Stock's method and pyrolysis of diborane, reactions of diboranes with Lewis bases- symmetric and unsymmetric cleavage, types of bonds in higher boranes- the styx number, formulae for arriving at the number of 2-centre and 3- centre bonds in boranes, Wade's rules as applied to boranes, Geometrical and Lipscomb's semitopological structures of B_4H_{10}, B_5H_9, B_5H_{11}, B_6H_{10} and $B_{10}H_{14}$. Carboranes: classification, nomenclature, structures of CB_5H_9, $C_2B_4H_8$, $C_3B_3H_7$ and $C_4B_2H_6$. Metallocarboranes: preparation and structures. Borazines: Preparation, properties and structure. Difference in chemical properties between borazine and benzene, borazine derivatives (N& B substituted). Structure, preparation and applications of boron nitride. Phosphazenes: Classification, Cyclophosphazenes-$(NPCl_2)_3$and $(NPCl_2)_4$- preparation and structure, Linear polyphosphazenes- preparation and applications. Sulphur-nitrogen compounds: (S_xN_y: x=y, x≠y). Condensed phosphates – linear polyphosphates, long chain polyphosphates and metaphosphates.

<u>Silicates- Classification and structures of ortho, pyro, chain, cyclic, sheet and three dimensional silicates</u>.

4. ACIDS AND BASES 6 hrs

(Review of acid- base concepts– Bronsted, Lewis and solvent system definitions of acids and bases, generalized acid-base concept.)

Systematics of Lewis acid-base interactions: Drago - Wayland equation. Factors affecting strength of Lewis and Bronsted acid/base strengths with special emphasis on steric effects and solvation effects. HSAB concept- Pearson's principle, classification of acids and bases as hard and soft, Bronsted acid-base strength versus hardness and softness, symbiosis, theoretical basis of hardness and softness.

5. NONAQUEOUS SOLVENTS 4hrs

Chemistry in non-aqueous media – Classification of solvents, leveling effect, acid-base reactions in BrF_3, N_2O_4 and molten salts. Reactions in super critical fluids. Ionic liquids-preparation of 1-butyl-3-methylimidazolium hexafluorophosphate, properties and applications of ionic liquids.

REFERENCES

1. Inorganic Chemistry, M. T. Weller, J. P. Rourke, T. L. Overton and F.A. Armstrong, 7th edition, Oxford Univ. Press, (2018).
2. Inorganic Chemistry, Catherine E. Housecroft and Alan G. Sharpe, 5th edition, Pearson Education Limited, (2018).
3. Principles of Inorganic Chemistry, B. W. Pfennig, 2nd edition, John Wiley & Sons Inc. (2022).
4. Inorganic Chemistry, G. L. Miessler, P. J. Fischer and D. A. Tarr, 5th edition, Pearson Education Limited, (2014).
5. Inorganic Chemistry, J. E. House, 3rd edition, Academic Press (2020).
6. Chemistry of the Non-Metals, R. Steudel, Walter de Gruyter GmbH (2020).
7. Fundamental concepts of Inorganic chemistry, 2nd edition Asim K Das, volume 1,.(2014).
8. Reactions in supercritical fluids- a Review, Bala Subramaniam and Mark A. McHugh Ind. Eng. chem. Process Design and development. Vol 25. Issue 1. Pages 1-12, (1986).
9. Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, J.E. Huheey, E.A. Keiter and R.L. Keiter, Okhil. K.Medhi, Pearson Education Asia Pvt. Ltd. (2006).
10. Basic Inorganic Chemistry - F.A. Cotton, G. Wilkinson and P. L. Gaus, John-Wiley and sons, III edition, (1995).

Semester	I
Paper Code	CH7221

Paper Title	ORGANIC CHEMISTRY - I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. STRUCTURE, REACTIVITY & REACTION MECHANISMS 11+4 =15 hrs

Resonance, field effects, hyperconjugation, steric effects and steric inhibition of resonance. Problem based on these concepts.

Quantitative treatment of field and resonance effects – Hammett and Taft equations.

Basic concepts of reaction mechanisms; thermodynamics and kinetics of reactions, Thermodynamic vs. kinetic control, Hammond postulate, microscopic reversibility, Marcus theory, Curtin – Hammett principle.

Reactive intermediates: Generation, structure, stability and reactivity of ***carbocations, carbanions, carbon free radicals***, carbenes and nitrenes.

Methods of determining mechanisms: Characterization of intermediates, kinetics, stereochemistry, kinetic isotopic effects, isotopic labeling experiments and solvent effects.

2. STEREOCHEMISTRY 15+2 = 17 hrs

Molecules with 2 and 3 stereocenters – Interconversion of perspective, Fischer, sawhorse and Newman structures. R-S notation of molecules with more than 2 chiral centers, erythro/threo nomenclature, meso compounds, systems with pseudoasymmetric centres.

Axial chirality – allenes, spiranes, biphenyls – R, S notation of these systems. Planar chirality – ansa compounds, cyclophanes, P, M notations. Helicity – helicenes, end substituted benzphenanthrenes. ***Classification of racemic modifications, E-Z configuration notation. In-out isomerism***.

Homotopic, enantiotopic and diastereotopic atoms, groups and faces; prochirality; *pro-R/S, Re/Si* configuration notations.

Conformations of mono and di-substituted ethanes. Energy profiles of conformations of ethane, propane, butane and cyclohexane. Conformations of mono-substituted cyclohexanes, conformation and configurational details of di-substituted cyclohexanes.

Fused rings and bridged rings, nomenclature of bridged systems, decalins, norbornanes, bicyclo [2.2.2] octane.

3. ALIPHATIC NUCLEOPHILIC SUBSTITUTION 11 hrs

Substitution at sp^3 carbon atom; limiting cases- S_N1 and S_N2 mechanisms. Factors influencing S_N1 and S_N2 reactions – substrate, leaving group, nucleophile and solvent. Ambident substrates and nucleophiles – regioselectivity. Borderline cases: intermediate mechanism, mixed S_N1 and S_N2 mechanism. Neighboring group participation, non-classical carbocations. S_Ni mechanism. Allylic rearrangements.

Substitution at a trigonal carbon atom – the tetrahedral mechanism, formation of acid derivatives, cleavage of esters and N-acylation reactions. Substitution at vinyl carbon - tetrahedral and addition-elimination mechanisms.

4. ELIMINATION REACTIONS 6 hrs

The E2, E1, E1cB and E2C mechanisms and the spectrum of elimination mechanisms. Regioselectivity and stereochemistry of E2 and E1 reactions. Factors influencing E1, E1cB and E2 reactions – substrate, leaving group, nucleophile and solvent. Substitution vs. elimination. Pyrolytic eliminations: Hofmann elimination, elimination in esters, xanthates and N–oxides - mechanisms and orientation.

5. AROMATIC SUBSTITUTION 9+2=11 hrs

Resonance and molecular orbital interpretation of aromaticity of benzene. Hückel's rule- aromaticity and anti-aromaticity. Aromaticity/anti-aromaticity of benzenoid and non-benzenoid systems and ions.

Electrophilic substitution: Mechanistic interpretations of second substitution, orientation and reactivity, ortho/para ratio, ipso attack. Orientation in third substitution. Orientation and reactivity of other ring systems - polycylic aromatic hydrocarbons (naphthalene, anthracene, phenanthrene), heterocyclic systems (pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyrimidine, purine and indole). ***Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction***.

Nucleophilic substitution: S_NAr, S_N1, benzyne and SR_N1 mechanisms.

Reactivity in arenes – effect of substrate structure, leaving group and nucleophile. Reactivity of heterocyclic systems (pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyrimidine, purine and indole). von Richter and Smiles rearrangements.

REFERENCES

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, And Structure, Michael B. Smith and Jerry March, 7th Edn, John Wiley& Sons Inc.

2. Organic Chemistry, Clayden, Greeves, Warren and Wothers, Oxford University Press, (2001).

3. Guidebook to Mechanism in Organic Chemistry (6^{th} Edition), Peter Sykes, Pearson Education Limited, (1986).

4. Stereochemistry of Carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Mander, John Wiley, (1994)

5. D. Nasipuri, Stereochemistry of Organic Compounds, Wiley Eastern, New Delhi, (1991).

6. Advanced Organic Chemistry, Part A, F. A. Carey and J. Sundberg, 5^{th} Edn.,Springer, (2007).

7. Organic chemistry, Volumes I and II, I. L. Finar, Longman, (1999).

Semester	I
Paper code	CH7321

Paper title	PHYSICAL CHEMISTRY – I (Quantum Chemistry)
Number of teaching hrs per week	3
Total number of teaching hrs per semester	45
Number of credits	3

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. QUANTUM MECHANICS FORMALISM 7 hrs

(*Emergence of quantum mechanics: black body radiation, photoelectric effect and Bohr's model of H-atom*)

Matter–wave duality, de Broglie equation; Heisenberg's uncertainty principle; time–independent Schrödinger equation from the equation of a standing wave; physical meaning of wave function, well-behaved wave functions; normalization and orthogonality of wavefunctions.

Operators and operator algebra; eigen value equations, eigen functions and eigen values; hermitian operators and their properties; postulates of quantum mechanics; time–dependent Schrödinger equation.

2. QUANTUM MECHANICAL TREATMENT OF SIMPLE SYSTEMS 11 hrs

Quantum mechanical treatment of a free particle and a particle in a 1D/3D potential well; eigen values and normalized eigen functions, nodes, symmetry and antisymmetry of eigen functions; quantum mechanical degeneracy (cubic well); accidental degeneracy (tetragonal and orthorhombic wells); application of particle in a 1D potential well model to conjugated systems; quantum mechanical tunneling (no derivation) and examples.

Quantum mechanical treatment of harmonic oscillator, eigen values and normalized eigen functions, zero point energy.

Quantum mechanical treatment of a particle on a ring and rigid rotator; eigen functions and eigen values; quantization of angular momentum.

Quantum mechanical treatment of hydrogen atom; eigen values and orbital functions; expressions of orbital functions in atomic units; radial and angular plots.

3. APPROXIMATE METHODS AND MULTIELECTRON ATOMS 8 hrs

Variation theorem and its proof; application to the ground state of helium atom.

Perturbation theory (time-independent); application of perturbation method to the ground state of helium atom (first order correction only).

Multielectron atoms – symmetric and antisymmetric wave functions; ground and excited states of helium; spin orbitals and Pauli principle; Slater determinants; self-consistent field (SCF) method; Hartree-Fock SCF method; Slater orbitals; effective nuclear charge based on Slater's rules.

4.THEORY OF ANGULAR MOMENTUM 6 hrs

Commutation relationships among angular momentum operators; quantum mechanical definition of angular momentum; ladder operators; deriving eigen values of the generalized angular momentum operators using ladder operators.

Orbital and spin angular momenta; spin-orbit interaction; coupled and uncoupled representation of angular momenta of composite systems; coupling of several angular momenta; term Symbols, L-S coupling (Russel–Saunders Coupling), and j-j coupling; Hund's rule of maximum stability.

5. CHEMICAL BONDING 13 hrs

Diatomic molecules: Born-Oppenheimer approximation.

MO theory: LCAO–MO approximation; hydrogen molecule ion (H_2^+); hydrogen molecule; limitations of MO treatment; excited states of H_2 – singlet and triplet states.

Valence bond theory: hydrogen molecule ion (H_2^+); hydrogen molecule (Heitler–London theory).

Hückel MO treatment for simple π–systems – ethylene, propenyl and cyclopropenyl systems, *butadiene, cyclobutadiene, benzene. Inroduction to extended Hückel calculations.*

REFERENCES

1. Quantum Chemistry, R. K. Prasad, New Age International (P) Ltd (2010).

2. Quantum Chemistry, D. A. McQuarrie, Viva Books Pvt Ltd (2003)

3. Quantum Chemistry, I. N. Levine, Prentice Hall India (2001).

Semester	I
Paper code	CH7421
Paper title	SPECTROSCOPIC METHODS OF ANALYSIS - I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. GROUP THEORY IN CHEMISTRY 17 hrs

Symmetry elements and symmetry operations, definition of groups and subgroups, simple theorems in group theory and group multiplication tables. Conjugate relationships, classes of operations and order of a group. Symmetries with multiple higher order axis-symmetry operations in tetrahedral and octahedral point groups. Improper axis of symmetry - operations generated by S_n axis, symmetry conditions for molecular chirality. Point groups, Schoenflies notations for point groups, representation of symmetry operations as matrices, reducible and irreducible representations, characters of representations, great orthogonality theorem (without proof) and its corollaries, properties of irreducible representations. Mulliken's symbols for irreducible representations. Character tables - character tables of C_{nv}, C_{nh} D_{nh} and C_n point groups (derivation of character table only for C_{2v} and C_{3v} point group). Applications of character tables in IR and Raman.

Group theory & Quantum mechanics: wave functions as basis for irreducible representations, direct products, time dependent perturbation theory, transition moment integral and selection rules in spectroscopy.

2. MICROWAVE SPECTROSCOPY 8 hrs

Rotations of molecules, rigid diatomic molecule-rotational energy expression, energy level diagram, selection rules, expression for the energies of spectral lines, computation of intensities, effect of isotopic substitution, centrifugal distortion and the spectrum of a non-rigid rotor. Rotational spectra of polyatomic molecules - linear, and symmetric top molecules. Calculation of bond length of diatomic and linear triatomic molecules. Stark effect.

3. INFRARED SPECTROSCOPY 14 hrs

Vibrations of molecules, harmonic and anharmonic oscillators-vibrational energy expression, energy level diagram, selection rules, expression for the energies of spectral lines, fundamentals, overtones, hot bands, vibrational frequency, force constant, effect of isotopic substitution. Diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational-rotational spectra of diatomic molecules, P, Q and R branches, breakdown of the Born-Oppenheimer approximation. Vibrations of polyatomic molecules: Normal coordinate, translations, vibrations and rotations, vibrational energy levels, fundamentals, overtones and combinations. Vibration-rotation spectra of polyatomic molecules, parallel and perpendicular vibrations of linear and symmetric top molecules.

4. RAMAN SPECTROSCOPY 8 hrs

Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of Raman effect, pure rotational Raman spectra of linear and symmetric top molecules, vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure – O and S branches, Polarization of Raman scattered photons, Structure determination from Raman and IR spectroscopy - AB_2 and AB_3 molecules.

5. ELECTRONIC SPECTROSCOPY 13 hrs

Vibrational coarse structure, intensities by Frank-Condon principle, dissociation energy, rotational fine structure, Fortrat diagram, Pre-dissociation.

Electronic structure of diatomic molecules-basic results of MO theory, Classification of states by electronic angular momentum, molecular orbitals, selection rules, spectra of singlet and triplet molecular hydrogen.

Application of group theory to the spectra of $CH_2 = CH_2$ and benzene.

Decay of excited states-radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion (Jablonski diagram).

REFERENCES

1. Chemical Applications of Group Theory, F.A. Cotton, Wiley Eastern (2009).
2. Introduction to Molecular Spectroscopy, C.N. Banwell & M.McCash, TMH Pub (2010).
3. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (Int. Students Edition) (1988).
4. Molecular Spectroscopy, J.D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
5. Modern Spectroscopy, J.M. Hollas, John Wiley (2010).
6. Vibrational Spectroscopy, D.N. Sathyanarayana, New Age International (P) Ltd. (1996).

7. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, (2001).

8. A simple approach to group theory in chemistry. S. Swarnalakshmi, T Saroja and R M Ezhilarasi. Universities Press. ISBN: 9788173716232, 9788173716232

10. Group Theory And Its Chemical Applications. ISBN: 9351428443, Himalaya Pub. House-New Delhi (2014).

Semester	I
Paper code	CH7521
Paper title	PRINCIPLES OF CHEMICAL ANALYSIS
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. ERRORS IN CHEMICAL ANALYSIS, STATISTICAL DATA TREATMENT AND EVALUATION 12+1=13 hrs

Significant Figures: Rounding of numbers. Addition and subtraction; multiplication and division.

Errors: Some important terms: replicate, outlier, accuracy, and precision. Errors affecting precision and accuracy; ***systematic errors*: *sources and types of systematic errors with examples***. Ways of expressing accuracy: absolute and relative errors; constant and proportional errors. ***Detection of systematic instrument and personal errors***. Identification and compensation of systematic method errors. Terms used to describe precision of a set of replicate measurements. Mean and median. Deviation and average deviation from the mean.

Statistical treatment of random errors; spread, sample, and population; sample mean and population mean. Standard deviation and variance of population; Gaussian distribution. Propagation of determinate errors. Sample standard deviation, sample variance, standard error of the mean, relative standard deviation, coefficient of variation, pooled standard deviation. Statistical data treatment in scientific calculations. Confidence interval.

Student - t statistics, significance testing, null hypothesis, one tailed and two tailed significance tests. Comparing measured results with a known value.

Comparison of two experimental means. Comparison of standard deviation with F-test. Paired t-test for comparing individual differences. Error in hypothesis testing. Criteria for rejection of an observation- Q test. Quality assessment: control charts. Calibration curves: least square method. Finding the least square line. Expression for slope, intercept, standard deviation about regression. Standard deviation of the slope and intercept. Coefficient of determination. Calibration sensitivity, Analytical sensitivity, Linear dynamic range, limit of quantisation, limit of detection.

Method validation: determination limits, calibration sensitivity. Limit of quantization and linear dynamic range.

2. ACID – BASE TITRATIONS 8 hrs

Basic principles: pH scale, dissociation constants of acids and bases. Titration curves for monobasic acids, pH calculations, theory of indicators. Titration curves for di, tri basic acids, amino acids, and bases. Fractions of phosphoric acid species as a function of pH. Gran's plots. Application of acid-base titrations for environmental, clinical, nutritional and industrial estimations.

Acid–base titrations in non-aqueous solvents –acid base window, acidic and basic titrants, methods of titration. Titrations in glacial acetic acid and ethylene diamine, applications of non-aqueous titrations.

3. REDOX TITRATIONS 8 hrs

Nernst equation, standard and formal potentials. Titration curves, end point signals, indicators, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponent systems. Adjustment of analyte's oxidation state. Application of oxidants such as permanganate, dichromate, cerium (IV), bromates, iodates, and reductants such as ferrous ammonium sulphate and ascorbic acid. Application for environmental, clinical, nutritional and industrial estimations.

Karl-Fischer titrations: Stoichiometry of the reaction, preparation of the reagent, titration method, standardization of the reagent using water-in-methanol, determination of water in samples, interference and their elimination, application to quantitative analysis of some organic compounds such as alcohols, carboxylic acids, acid anhydrides and carbonyl compounds.

4. PRECIPITATION TITRATIONS 4 hrs

Solubility product. Theoretical principles: titration curves, end point signals, Mohr, Volhard and adsorption indicators. Applications of argentometric titrations in estimation of F^-, K^+, CO_3^{2-}, $C_2O_4^{2-}$, acetylenes and mixture of halides.

5. COMPLEXOMETRIC TITRATIONS 7 hrs

Complexometric titrations involving monodentate and polydentate ligands, advantages of EDTA. Expressions for the different fractions of EDTA in solution as a function of pH, conditional stability constants, effect of pH and second complexing agent on the conditional stability constant and titration curve. Selectivity by pH control, masking and demasking, metal ion indicators, types of EDTA titrations, application of EDTA titrations for environmental, clinical, nutritional and industrial estimations.

6. GRAVIMETRIC ANALYSIS 4+1 = 5 hrs

Types of gravimetric analysis, different steps involved in gravimetric estimation. Formation and treatment of precipitates, factors determining successful precipitation, nucleation and size of the particles, properties of precipitating agents. Coagulation and peptization. Von Weimarns theory of relative supersaturation. Impurities in precipitates, co-precipitation, post precipitation. Methods of minimizing co-precipitation. Precipitation from homogeneous solution. Gravimetric factor. ***Important precipitating agents and their significance in inorganic analysis. Advantages and disadvantages of organic precipitants***.

7. KINETIC METHODS OF ANALYSIS 4+1 = 5 hrs

Equilibrium and kinetic methods. Classification of chemical kinetic methods. Rate laws, pseudo first order kinetics, Expression for pseudo first order kinetics, types of kinetic methods, Direct computation and curve fitting methods. One point and two point fixed time integral methods for the calculation of rate constant. Direct computation variable time integral methods. Differential reaction rate methods, initial rate methods. Enzyme catalysis, basis for substrate and enzyme determination. ***Applications of catalytic and non-catalytic kinetic methods.***

8. ABSORPTION AND EMISSION TECHNIQUES 6+1= 7 hrs

Quantitative aspects of spectrochemical measurements. Absorbance, molar absorptivity. Nephelometric and turbidimetric methods, choice of method and instrumentation. ***DU Pont model for turbidity; EEL nephelometer***. Analytical applications - turbidimetric titrations.

(Molecular luminescence- explanation for fluorescence and phosphorescence using Jablonski diagram)

Quantitative aspects of fluorescence. Interpretation- internal conversion, vibrational relaxation and inter system crossing. Variables that affect fluorescence and phosphorescence. Transition types in fluorescence. Fluorescence and structure, examples, effects of structural rigidity, temperature, dissolved oxygen and solvent. Effect of substitution on the benzene ring and fluorescence efficiency. Instrumentation.

Atomic absorption methods: principle and instrumentation (single and double beam), light sources of AAS, atomization (flame and electrothermal), interferences in AAS and corrections applied. Detection limits. ***Atomic emission method (AES), advantages and disadvantages, Plasma – ICP, ICP sources, DCP, and ICP-MS techniques***.

9. THERMAL METHODS OF ANALYSIS 3 hrs

Introduction to thermal methods. Principle, instrumentation, data analysis and applications of thermogravimetry, differential thermal analysis, differential scanning calorimetry and thermometric titrations.

REFERENCES

1. Fundamentals of Analytical Chemistry; Skoog, West. Holler and Crouch 9th edition; Mary Finch. (2014).
2. Principles of Instrumental Methods of Analysis; Skoog, Holler and Nieman, 5th edition, Saunders College Publishing, International Limited (1999).
3. Analytical Chemistry; Gary D Christian; 6th edition; John Wiley and Sons (2010).
4. Modern Analytical Chemistry; David Harvey; McGraw Hill Higher education publishers, (2000).
5. Analytical Chemistry Principles; John H Kennnedy, 2nd edition, Published by Cengage Delmar Learning India Pvt (2011).
6. Vogel's Text book of quantitative chemical analysis; 6th edition, Pearson Education Limited, (2007).

PRACTICALS

Semester	I
Paper code	CH7P1
Paper title	INORGANIC CHEMISTRY PRACTICAL I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

QUALITATIVE ANALYSIS: 11 Units

Semi-micro qualitative analysis of a mixture containing two familiar cations and anions each and one of the less familiar elements: W, Mo, Ce, Th, Zr, V, U and Li.

REFERENCES

1. Vogel's Textbook of Qualitative Chemical Analysis, J Bassett, R C Denny, G H Jeffery and J Mendham, ELBS (1986).
2. Vogel's Textbook of Quantitative Chemical Analysis, 5th edition, G N Jeffery, J Bassett, J Mendham and R C Denny, Longman Scientific and Technical (1999).
3. Inorganic semimicro Qualitative Analysis, V.V. Ramanujam, The National Publ. Co. (1974).

Semester	I
Paper code	CH7P2
Paper title	INORGANIC CHEMISTRY PRACTICAL II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

QUANTITATIVE ANALYSIS: **11 Units**

Volumetric and gravimetric determination of the following mixtures:
(a) Iron and aluminium (b) Copper and nickel (c) Copper and iron (d) Copper and zinc
(e) Barium and calcium.

REFERENCES

1. Vogel's Textbook of Qualitative Chemical Analysis, J Bassett, R C Denny, G H Jeffery and J Mendham, ELBS (1986).

2. Vogel's Textbook of Quantitative Chemical Analysis, 5th edition, G N Jeffery, J Bassett, J Mendham and R C Denny, Longman Scientific and Technical (1999).

3. Inorganic semimicro Qualitative Analysis, V.V. Ramanujam, The National Publ. Co. (1974).

Semester	I
Paper code	CH7P3
Paper title	ORGANIC CHEMISTRY PRACTICAL I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

I. QUALITATIVE ANALYSIS: **11 Units**

Separation, systematic analysis and identification of organic compounds in a binary mixture.

REFERENCES

1. Laboratory Manual of Organic Chemistry, Day, Sitaraman and Govindachari (1996).

2. Practical Organic Chemistry, Mann and Saunders (1980).

3. Textbook of Practical Organic Chemistry, A.I. Vogel (1996)

4. Textbook of Quantitative Organic Analysis, A.I. Vogel (1996).

5. A Handbook of Organic Analysis, Clarke and Hayes (1964).

Semester	I
Paper code	CH7P4
Paper title	ORGANIC CHEMISTRY PRACTICAL II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

II. QUANTITATIVE ANALYSIS: 11 Units

1. Determination of equivalent weight of carboxylic acids.
2. Saponification value of oil/fat.
3. Estimation of glucose.
4. Estimation of phenols by acylation method.
5. Iodine value oil/fat.
6. Estimation of nitro group.
7. Estimation of nitrogen Kjeldhal's method.
8. Estimation of carbonyl group by hydroxylamine- pyridine method.

REFERENCES

1. Laboratory Manual of Organic Chemistry, Day, Sitaraman and Govindachari (1996).
2. Practical Organic Chemistry, Mann and Saunders (1980).
3. Textbook of Practical Organic Chemistry, A.I. Vogel (1996)
4. Textbook of Quantitative Organic Analysis, A.I. Vogel (1996).
5. A Handbook of Organic Analysis, Clarke and Hayes (1964).

SECOND SEMESTER

THEORY PAPERS

Semester	II
Paper Code	CH8121
Paper Title	INORGANIC CHEMISTRY – II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. METAL – LIGAND BONDING 11+4=15 hrs

<u>(Review of basic concepts of co-ordination chemistry)</u>. Geometries of complexes with coordination nos. 2 to 12. Crystal field theory: crystal field splitting in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal ligand fields; structural and thermodynamic effects of crystal field splitting; octahedral ionic radii, Jahn–Teller distortion in metal complexes and metal chelates, hydration and lattice energies, site preferences in spinels, octahedral versus tetrahedral co-ordination, Irving-William stability order; spectrochemical series; limitations of crystal field theory. Evidences for metal– ligand orbital overlap from ESR, NMR, electronic spectra and antiferromagnetic coupling; nephelauxetic effect and nephelauxetic series. Ligand Field Theory, Ligand Group of Orbitals. MO theory : symmetry adapted linear combinations of Atomic Orbitals, MO diagrams of octahedral complexes (including π-bonding). ***<u>MO energy level diagrams in tetrahedral complexes</u>*** .

2. METAL – LIGAND EQUILIBRIA IN SOLUTION 8 hrs

Step-wise and overall formation constants and their relationships, trends in step-wise formation constants and exceptions to the trends; factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate and macrocyclic effects and their thermodynamic origin; kinetic and thermodynamic stability of metal complexes.

Determination of composition and stability constants of complexes by spectrophotometry (Job's method) and potentiometry.

4. VIBRATIONAL SPECTRA OF TRANSITION METAL COMPLEXES 4 hrs

Changes in the IR spectra of donor molecules upon coordination, Change in spectra accompanying change in symmetry upon coordination; Oxo anions as ligands; Different binding modes of NO_2^-, NO_3^-, SO_4^{2-} and ClO_4^-.

5. ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES 12 hrs

Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel and Tanabe-Sugano diagrams, Correlation diagram of d^2 configuration, spectra of 3d metal aqua complexes of trivalent V, Cr, divalent Mn, Co, Ni, and $[CoCl_4]^{2-}$, calculation of Dq, B and β parameters, charge transfer spectra, spectral behaviour of lanthanide ions.

6. MAGNETIC PROPERTIES OF METAL COMPLEXES 8+1=9 hrs

Origin and types of magnetic behaviour; diamagnetism, paramagnetism, ferromagnetism and antiferromagnetism, magnetic susceptibility and its measurement by the Guoy method and the ***Faraday method***, temperature dependence of magnetism – Curie and Curie-Weiss laws, types of paramagnetic behaviour; spin-orbit coupling, magnetic behaviour of lanthanide ions, quenching of orbital contribution and spin only behaviour (explanation based on A, E and T terms), applications of magnetic data, temperature independent paramagnetism, spin-cross over.

7. STRUCTURE AND BONDING IN SELECTED METAL COMPLEXES 10+2=12h

Hydride, dihydrogen, isocyanide complexes; mononuclear and dinuclear metal carbonyls and metal carbonyl clusters, ***Wade's rules as applied to metal carbonyl clusters***, nitrosyl, dinitrogen and tertiary phosphine complexes, ligand cone angle in phosphine complexes; ***CO_2, SO_2 and dioxygen complexes***.

Stereochemical non-rigidity, Stereoisomerism – chirality, optical activity, Circular Dichroism, Optical Rotatory Dispersion, Cotton effect and absolute configurations.

REFERENCES

1. Advanced Inorganic Chemistry, F.A Cotton and G. Wilkinson, John Wiley & Sons Inc., 6th edition, (1999).
2. Advanced Inorganic Chemistry – A Comprehensive Text, F.A. Cotton and G. Wilkinson, Wiley Eastern limited, III edition, (1972).

3. Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, J.E. Huheey, E.A. Keiter and R.L. Keiter, Pearson Education Asia Pvt. Ltd. (2000).
4. Physical Methods in Inorganic Chemistry, Russell S. Drago, Litton Educational Publishing Inc. (1965).
5. Inorganic Chemistry, 7th Edition, M. Weller, J. Rourke, T. Overton and F. Armstrong, Oxford Univ. Press. (2018).
5. Inorganic Chemistry, G. Wulfsberg, Viva Books Pvt. Ltd. (2002).
6. Inorganic Chemistry, G.L. Miessler and Tarr, 5th edition, Pearson Education Ltd. (2014).
7. Coordination Chemistry, 2nd edition, D. Banerjea, Asian Books Pvt. Ltd. (2007).
8. Physical Inorganic Chemistry, S. F. A. Kettle Springer-Verlag GmbH(1996).
9. Inorganic Chemistry, 4th Edition, C. E. Housecraft and A. G. Sharpe, Pearson Education Ltd. (2012).

Semester	II
Paper Code	CH8221
Paper Title	ORGANIC CHEMISTRY – II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. ADDITION REACTIONS **10 hrs**

Addition to carbon-carbon multiple bonds: mechanisms of electrophilic addition reactions; regioselectivity and stereoselectivity; hydrogenation and hydroboration; Nucleophilic addition: Michael addition, mechanisms of formation of hydrates, acetals, oximes and hydrazones of carbonyl compounds, Wittig reaction.

Addition to carbon-hetero atom multiple bonds: mechanisms of metal hydride reduction of carbonyl compounds and nitriles. <u>***Addition of Grignard reagents and organolithium reagents to carbonyl compounds***</u>

2. ALIPHATIC ELECTROPHILIC SUBSTITUTION **5 hrs**

S_E2, S_E1 and S_Ei mechanisms, hydrogen exchange, migration of double bonds. Aliphatic diazonium coupling, nitrosoation at carbon and nitrogen, diazo transfer reaction, carbene and nitrene insertion, decarboxylation of aliphatic acids; Haller-Bauer reaction.

<u>***Halogenation of aldehydes, ketones and acids, haloform reaction***</u>**.**

3. REARRANGEMENTS **15 hrs**

Carbon to carbon migrations: Wagner-Meerwein, pinacol-pinacolone, benzil-benzilic acid, Favorskii and Neber rearrangements; Arndt-Eistert synthesis; expansion and contraction of rings.
Carbon to nitrogen migrations: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangements.
Nitrogen/oxygen/sulfur to carbon migrations: Stevens and Wittig rearrangements.
Carbon to oxygen migrations: Baeyer-Villiger rearrangement.
Non-1,2 rearrangements: Fischer indole synthesis, benzidine rearrangement.

4. PERICYCLIC REACTIONS 20 hrs

Molecular orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene. Meaning of HOMO, LUMO, bonding, antibonding and nonbonding molecular orbitals.

Molecular orbital symmetry; frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems; classification of pericyclic reactions. Theories to rationalize pericyclic reactions: Woodward-Hoffmann orbital Symmetry Correlation Diagram, Frontier Molecular Orbital approach (FMO), Woodward-Hoffmann rules, Hückel-Mobius (Perturbation Molecular Orbital or Transition State Aromaticity) method.

Electrocyclic reactions: conrotatory and disrotatory modes; 4n, 4n+2 and allyl systems. Cycloadditions: suprafacial and antarafacial additions, 4n and 4n+2 systems; [2+2] addition of ketenes, 1,3-dipolar cycloadditions and chelotropic reactions.

Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 1,3-, 1,5-, 3,3-, and 2,3-sigmatropic rearrangements; Cope and Claisen rearrangements; Sommelet-Hauser rearrangement; Alder-Ene reaction.

5. FREE RADICAL REACTIONS AND PHOTOCHEMISTRY 10 hrs

(*Review/recall: Homolysis of bonds, photochemical excitation of molecules, Beer-Lambert's law, dissipation of energy - Jablonsky diagram*).

Generation of free radicals – thermolysis and photolysis of peroxides, peresters and azo compounds, hydrogen abstraction, chain process.

Free radical addition, substitution, elimination, rearrangement and electron transfer reactions. Use of free radicals in organic synthesis.

General principles of photochemistry: singlet and triplet states-differences in reactivity, photosensitisation; quantum efficiency, quantum and chemical yields.

Photochemical reactions: Norrish type I and type II cleavages, cis-trans isomerisation, di-π-methane rearrangement; Paterno-Buchi reaction; photoreduction of ketones; photochemistry of arenes.

REFERENCES

1. March's Advanced Organic Chemistry, Michael B. Smith and J. March, 6th Edn., John Wiley, (2007).
2. Advanced Organic Chemistry, Part A and B, F. A. Carey and J. Sundberg, 5th Edn., Plenum press, (2007).
3. Organic Chemistry, Paula Yurkanis Bruice, 7th Edn., Pearson Education, Inc., (2014).
4. Organic Chemistry, Seyhan Ege, 3rd Edn., Houghton Miftlin Company, (1999).
5. Frontier orbitals and Organic chemical reactions, Ian Fleming, John Wiley, (1980).

6. Radicals in Organic synthesis, B. Giese, Pergamon Press, (1986).
7. Organic Photochemistry, J.M. Coxon and B. Halton, 1st Edn., Cambridge University Press, London, (1974).
8. Molecular reactions and Photochemistry, C.H. Deputy and D.S. Chapman, 1st Edn. Prentice Hall India, New Delhi, (1972).
9. Mechanism and Theory in Organic Chemistry (3rd Edition), Thomas H. Lowry,Thomas H. Lowry (Author) Kathleen S. Richardson, Harper & Row: New York. (1987).
10. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory, S. Sankararaman, Wiley VCH, 2005
11. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh, 4th Edn. New Age International Publishers,2019.

Semester	II
Paper Code	CH8321
Paper Title	PHYSICAL CHEMISTRY – II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1 STATISTICAL THERMODYNAMICS 15+2 hrs

Introduction: Objectives of statistical thermodynamics, inputs from quantum mechanics and spectroscopy , system in terms of energy levels and population, thermally available energy levels, micro and macro states and their representation, distinguishable and indistinguishable particles, configuration and its weight, dominant configuration, ensemble and its types, ensemble averaging, Stirling's approximation, thermodynamic probability, its relationship with entropy, postulates of statistical thermodynamics.

Maxwell Boltzmann statistics: assumptions, derivation of equation for fraction of molecules occupying a given energy range, partition function and its physical significance.
Bose-Einstein statistics: assumptions, <u>***derivation of equation for fraction of molecules occupying a given energy range***</u>.
Introduction to quantum statistics, Fermi-Dirac statistics: assumptions, <u>***derivation of equation for fraction of molecules occupying a given energy range***</u>.
Partition function and thermodynamic parameters – derivation of expressions for internal energy, heat capacity, free energy, chemical potential, pressure, entropy and equilibrium constant. Derivation of translational/rotational/vibrational/electronic partition functions. Sackur-Tetrode equation.
Evaluation of partition functions from spectral data, thermodynamic properties of molecules from partition functions.

Application of statistical thermodynamics: equipartition theorem, heat capacity behavior of crystals

2. CHEMICAL THERMODYNAMICS **15 hrs**

Introduction –Review of thermodynamic laws and their significance.

Thermodynamics of open systems, Partial molal quantities: partial molal volume, partial molal free energy, chemical potential, effect of temperature and pressure on chemical potential, Gibbs-Duhem equation, chemical potential of a pure substance, fugacity, chemical potential in an ideal gas mixture. Experimental methods for the determination of fugacity.

Activity and activity coefficients: determination by solubility and emf methods, effect of temperature and pressure on fugacity and activity. Gibbs-Duhem-Margules equation – derivation and applications; Konovalov's first law and second law.

Chemical potential in ideal solution. Thermodynamic deduction of Henry's law, Raoult's law, Nernst distribution law, Phase rule and their validation. Chemical potential of non-ideal solutions; thermodynamics of mixing of ideal and non-ideal solutions. Excess thermodynamic functions.

3. NON-EQUILIBRIUM THERMODYNAMICS **8 hrs**

Irreversible processes and steady state. Conservation of mass and energy in open systems. Fluxes and forces Entropy production – entropy production due to heat flow. Entropy production and it's rate in matter flow. Microscopic reversibility and Onsagar's reciprocity relations. Phenomenological equations. Entropy production in terms of fluxes and forces. Entropy production and its rate in chemical reactions.

4. REACTION KINETICS **16 + 2 hrs**

Arrhenius and bimolecular collision theories. Activated complex theory – derivation of expression for rate constant by thermodynamic method and partition function method. Reactions in solutions – factors affecting reaction rates in solutions.

Diffusion controlled reactions – influence of solvation, internal pressure and dielectric constant on reaction rates. Ionic reactions – double sphere model for effect of solvent on ionic reaction rates. Diffusion controlled reactions.

Primary and secondary salt effects.

Kinetic and thermodynamic control of reactions.

Unimolecular reactions – quantitative treatment of Lindemann and Hinshelwood theories, qualitative treatment of RRK and RRKM theories, comparison of these theories.

Kinetics of chain reactions – H_2 and O_2 reaction – Explosion limits. Dehydrogenation of ethane, pyrolysis of acetaldehyde - Rice - Herzfeld mechanisms.
Kinetics of fast reactions, features of fast reactions.

Study of fast reactions by flow method, relaxation method, flash photolysis and NMR method.

5. KINETICS OF POLYMERIZATION **4 hrs**

Kinetics and mechanism of free radical polymerization, kinetic chain length and chain transfer. Kinetics of cationic and anionic polymerization. Co-polymerization – free radical mechanism, copolymer composition.

REFERENCES

1. Physical Chemistry, P.W. Atkins, Julio de Paula, W.H. Freeman and company, 9th edition (2010).
2. Chemical Kinetics, K.J. Laidler, Pearson Education (Singapore) Pvt. Ltd. 3rd Edition, (2004).
3. Advanced Physical Chemistry, J. N. Gurtu and A. Gurtu, Pragati Prakashan, 8th edition, (2006).
4. Textbook of Physical Chemistry, H.K. Moudgil, PHI Learning Pvt. Ltd., New Delhi, (2010)
5. Principles of Physical Chemistry, B.R. Puri, L. R. Sharma and M. S. Pathania, Vishal Publishers co. (2017).
6. Molecular thermodynamics, Donald A. McQuarrie, John D. Simon University Science Books, California, (1999).
7. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, New age International (P) Ltd. Publishers. First edition. Reprint (2012).
8. Thermodynamics, Rajaram and J. Kuriacose, Shobhanlal Publishers (1999).

Semester	II
Paper Code	CH8421
Paper Title	SPECTROSCOPIC METHODS OF ANALYSIS – II
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. UV AND VISIBLE SPECTROSCOPY 6 hrs

Nature of electronic transitions; the origin of UV band structure; principles of absorption spectroscopy, instrumentation and presentation of spectra. Solvents; terminology: chromophores; auxochromes; bathochromic shift; hypsochromic shift, hyperchromic shift, hypochromic shift. Effect of conjugation on the spectra of alkenes. Woodward – Fieser rules for polyenes. Electronic spectra of carbonyl compounds. Effect of solvent on $\pi - \pi^*$ and $n - \pi^*$ transitions. Woodward's rules for enones.

2. INFRARED SPECTROSCOPY 8 hrs

Infrared portion of electromagnetic spectrum. Energy, frequency, wave number relationship. Infrared absorption process. Principle of IR analysis, Uses of infrared spectrum. Modes of stretching and bending vibrations. Bond properties and absorption trends. Instrumentation of IR spectrometer: Dispersive and Fourier transform spectrometers. Preparation of samples for IR analysis. Analysis of an IR spectrum at a glance. Survey of functional groups with examples. Hydrocarbons: alkanes, alkenes and alkynes, aromatic hydrocarbons: Detailed discussions on C – H vibrations, C = C vibrations, conjugate effects and Ring size effects (internal bonds) = C – H bending vibrations (in alkenes and aromatic compounds – discussion on substitution patterns). Alcohols and phenols, ethers: Detailed discussion on O – H stretching vibration, effect of hydrogen bonding (effect of solvent polarity and concentration). Carbonyl compounds: Normal base values for C = O stretching vibrations for carbonyl compounds. Effect of electron withdrawing groups, inductive, resonance, hydrogen bonding, conjugation, ring size. General discussions of IR absorption characteristics of aldehydes, ketones, carboxylic acids, esters ketones and amides, acid anhydrides and chlorides. IR spectra of nitriles and phosphorous compounds, structure determination of simple molecules.

3. NMR SPECTROSCOPY 17 hrs

Nuclear spin states; nuclear magnetic moments; absorption of energy; mechanism of absorption (resonance). Population densities of nuclear spin states; The Chemical Shift and shielding; The Nuclear Magnetic Resonance Spectrometer -The Continuous-Wave (CW) Instrument and the Pulsed Fourier Transform (FT) Instrument. Chemical Equivalence; Integrals and Integration; Chemical environment and Chemical shift; Local Diamagnetic Shielding - Electronegativity Effects ; Hybridization Effects; Acidic and Exchangeable Protons; Hydrogen Bonding. Magnetic Anisotropy; Spin–Spin Splitting (n + 1) rule; origin of Spin–Spin Splitting; Pascal's Triangle. Low and high resolution spectra of ethanol – chemical exchange; NMR spectra of amides. The Coupling Constant; Solving NMR spectra problems. Coupling Constants: The Mechanism of Coupling - One-Bond Couplings (1*J*); Two-Bond Couplings (2*J*); Three-Bond Couplings (3*J*)- Karplus relationship. Long-Range Couplings (4*J*–*nJ*) ; Magnetic Equivalence .The Use of Tree Diagrams when the n + 1 Rule Fails; Measuring Coupling Constants from First-Order Spectra. Second-Order Spectra—Strong Coupling; First-Order and Second-Order Spectra; Spin System Notation; The A_2, AB, and AX Spin Systems; The AB_2 . . . AX_2 and A_2B_2 . . . A_2X_2 Spin Systems.

4. CARBON–13 NMR SPECTROSCOPY 7 hrs

The Carbon-13 Nucleus; Carbon-13 chemical shifts; Proton-Coupled C - 13 Spectra—Spin–Spin Splitting of Carbon-13 Signals. Proton-Decoupled C - 13 spectra; nuclear overhauser enhancement. Cross-Polarization: Origin of the nuclear overhauser effect; Problems with Integration in C - 13 spectra. Molecular relaxation processes; off-resonance decoupling. ***Combined spectral problems***.

5. ADVANCED NMR TECHNIQUES 5 hrs

Pulse widths, spins, and magnetization vectors. The DEPT experiment: number of protons attached to C - 13 atoms; determining the number of attached hydrogens. Introduction to two-dimensional spectroscopic methods; The COSY technique: ^1H-^1H correlations; an overview of the COSY experiment.

How to read COSY spectra. ***Problem solving***.

6. MASS SPECTROMETRY 8 hrs

Principle of mass spectrometry, mass spectrometer, resolution mass spectrum, molecular ion peak, base peak, fragment ion peaks, meta stable ion peak, isotope peaks, Nitrogen rule - definition and their significance. Determination of molecular weight and molecular formula. Carbocation: stability, types of fragmentation patterns: single bond, multiple bonds, McLafforty rearrangement, retro Diels-Alder. General discussions on the fragmentation patterns of alkanes, alkenes, aromatic hydrocarbons, alcohols, phenols, ethers, aldehydes, ketones, esters, carboxylic acids, amines. Different ionization and analysis methods: EI, CI, FAB, MALDI, etc. Structure determination of molecules.

7. ELECTRON PARAMAGNETIC RESONANCE SPECTROSCOPY 6 hrs

Principles. Presentation of ESR spectrum, DPPH as an external standard, significance of g values. hyperfine splitting, hyperfine coupling constants, EPR spectrum of hydrogen atom, isotropic systems involving more than one nucleus (same and different kinds)I = ½, 1, 3/2, 5/2. , (H, N, Co, Mn, V). Anisotropy in hyperfine coupling, EPR of triplet states, EPR spectra of transition metal ion complexes: Kramer's rule, interpretation of g – values, d^1 – d^5 systems. zero field splitting, EPR spectra of Mn^{2+} doped into MgV_2O_6. ENDOR and ELDOR techniques.

8. MOSSBAUER SPECTROSCOPY: (explanation using Sn and Fe compounds) **3 hrs**

Principle of analysis, significance of Doppler shift and recoil energy. Procedure for obtaining MS spectra, chemical shift or centre shift/ isomer shift, quadrupole shifting. Magnetic splitting, applications of MS.

REFERENCES

1. Physical methods in Inorganic chemistry, R.S. Drago, Affiliated East-West Press Pvt. Ltd., New Delhi (1965).
2. Infrared Spectra of Inorganic and co-ordination Compounds, K. Nakamoto, Wiley-Interscience, New York, (1970).
3. Vibrational spectroscopy: theory and Applications, D.N. Sathyanarayana, New-Age International Publishers, New Delhi (2000).
4. Electronic Absorption Spectroscopy and related techniques, D.N. Sathyanarayana, Universities Press, Bangalore, (2001).
5. Applications of absorption Spectroscopy to Organic Compounds, J.R. Dyer, Prentice – Hall, New Delhi, (1969).
6. Organic Spectroscopy, W. Kemp, ELBS London, (1975).
7. Spectrometric Identification of Organic Compounds, R.M. Silverstein and W.P. Webster, Wiley & Sons, (1999).
8. Organic Mass Spectroscopy, K.R. Dass and E.P. James, IBH New Delhi, (1976).
9. Mass Spectrometry of Organic Compounds, H. Budzkiewicz, Djerassi C. and D.H Williams, Holden-Day, New York, (1975).
10. Principles of Instrumental Analysis, D.A. Skoog, S.J. Holler, T.A. Nilman, 5th Edition, Saunders College Publishing, London, (1998).

11. Introduction to Spectroscopy, 5th Edition, Donald L. Pavia, Gary M. Lampman and George S. Kriz and James R. Vyvyan. Cengage Learning (2015).
12. Physical Methods for Chemists, R.S. Drago, 2nd Edition, Saunders College Publishing New York, (1992).
13. Mass Spectrometry – Analytical Chemistry By Open Learning -, R. Davies, M. Frearson and E. Prichard, John Wiley and Sons, New York, (1987).
14. Modern NMR techniques For Chemistry Research, Vol. 6, A.E. Derome, Oxford Pergamon Press, (1987).
15. Spectroscopic Methods in Organic Chemistry, 4th Edition, D.H. Williams and I. Fleming, Tata-McGraw Hill Publications, New Delhi, (1988).

Semester	II
Paper Code	CH8521
Paper Title	Separation Techniques
Number of teaching hours per week	3
Total number of teaching hours per semester	45
Number of credits	3

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. SOLVENT EXTRACTION **7 hrs**

Partition coefficient. Equation for batch extraction and multiple extraction. Extraction efficiency - pH effects. Extraction with metal chelator and crown ethers. Multistage extraction. Supercritical fluid extraction.

2. THEORETICAL ASPECTS OF CHROMATOGRAPHY **6 hrs**

Types of chromatography. Theoretical principles - retention time, retention volume, adjusted retention time, relative retention, capacity factor. Relation between retention time and partition coefficient. Scaling up, scaling rules. Efficiency of separation, resolution. Ideal chromatographic peaks (Gaussian peak shape). Diffusion, diffusion coefficient. Plate height - Plate height as a measure of column efficiency, number of theoretical plates. Asymmetric peaks. Factors affecting resolution. Band spreading - van Deemter equation, multiple paths, longitudinal diffusion, mass transport. Isotherms and the resulting band shapes.

3. GAS CHROMATOGRAPHY **7+1 hrs**

Separation process in gas chromatography: schematic diagram - packed column, open tubular columns and comparison with packed columns. Effect of column inner diameter and length of the column. Choice of liquid stationary phase: chiral phases for separating optical isomers, molecular sieves as stationary phase. Retention index, temperature and pressure programming, carrier gas, guard columns and retention gaps. Sample injections - split injection and spitless injection - solvent trapping and cold trapping, on column injection. Detectors - thermal conductivity detector, flame ionization detector, electron capture detector. Sample preparation for GC - solid phase microextraction, purge and trap, thermal desorption. Method development in GC. Derivatization in GC, GC-MS - selected ion monitoring. Applications.

<u>Nitrogen phosphorous detector, flame photometric detector, photoionization detector, Element specific plasma detectors.</u>

4. LIQUID CHROMATOGRAPHY 19 hrs

The chromatographic process - effect of small particles, scaling relation between columns. Relation between number of theoretical plates, particle size, column pressure. The column: stationary phase, bonded stationary phases, monolithic silica columns, solute column interactions - shape selectivity. The elution process - elution strength. Normal phase chromatography, reversed phase chromatography - isocratic and gradient elution, selecting the separation mode, solvents. Maintaining symmetric band shape, dead volume. Injection and detection in HPLC, pumps and injection valves, detector characteristics, signal to noise ratio, detection limits, linearity. Spectrophotometric detectors: refractive index detector, evaporative light scattering detector. Method development in HPLC, method development in reversed phase separation. Criteria for adequate separation, optimization with one organic solvent, optimization with two or three different organic solvents, temperature as a variable, choosing a stationary phase. Gradient separations - dwell volume and dwell time, developing a gradient separation. Derivatization of LC, LC-MS. Applications.

Ion Exchange chromatography: Ion exchangers, ion exchange selectivity, selectivity coefficient, Donnan Equilibrium, suppressed ion, anion and cation chromatography, ion chromatography without suppression, detectors. Ion pair chromatography. Chiral ion exchangers: chiral phases (amylose, crown ether, and cyclodextrins), chiral ligand exchange - pirkle brush type phases. Applications.

Molecular exclusion chromatography: The elution equation, stationary phase, molecular mass determination. Applications.

Affinity chromatography: Principle: matrix, ligand, spacer arm - properties required for efficient and effective chromatographic matrix, partial structure of agarose. Types of ligands - need of spacer arm. Immobilized metal affinity chromatography. Applications.

Supercritical Fluid Chromatography: Properties of supercritical fluids, instrumentation and operating variables. Effect of pressure, stationary phase, mobile phase, detectors. Applications.

5. Thin layer chromatography (1+1) hrs

Introduction, experimental techniques, preparation of thin layer plates, sample application, developing chromatogram, visualizing chromatogram, retention factor, high performance thin layer chromatography, forced flow planar chromatography. 2D TLC. Application of TLC.

6. Paper Chromatography 3 hrs

Introduction, principle, migration parameters. Types of paper chromatography: descending, ascending, ascending-descending, radial paper, two-dimensional chromatography. Experimental details for qualitative and quantitative analysis. Applications.

REFERENCES

1. Quantitative Chemical Analysis, Daniel C. Harris, 7th edition., (W. H. Freeman and Company, New York, (2006).

2. Analytical Chemistry Principles – John H Kennnedy, 2nd edition, Published by Cengage Delmar Learning India Pvt (2011).

3. Instrumental Methods of Chemical Analysis, Gurdeep R Chatwal, Sham K Anand, Himalaya Publishing House (2003).

4. Fundamentals of Analytical Chemistry, D. S Skoog, D. M. West, F. J. Holler, S. R. Crouch, 9th Edition, Cengage Learning (2014).

5. Principles of Instrumental Analysis, Skoog, Holler and Nieman, 5th edition, Saunders College Publishing, International Limited (1999).

6. Introduction to modern liquid chromatography, Lioyd R. Snyder, J J Kirkland, J W Dolan, 3rd edition, Wiley Publication (2010).

7. Principle and Techniques of Biochemistry and Molecular Biology, Walker Jon and Keith Wilson, 7th Edition, Cambridge University Press (2010).

PRACTICAL PAPERS

Semester	II
Paper Code	CH8P1
Paper Title	PHYSICAL CHEMISTRY PRACTICAL I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

Physical Chemistry Practical I

1. Determination of the velocity constant, catalytic coefficient, temperature coefficient, energy of activation and Arrhenius parameters for the acid hydrolysis of an ester by volumetry.
2. Kinetics of reaction between $K_2S_2O_8$ and KI (salt effect) by volumetry.
3. Determination of rate constant for the oxidation of alcohol by colorimetry.
4. Determination of partial molal volume of ethanol by reciprocal density method.
5. Determination of partial molal volume by apparent molar volume method, NaCl-H_2O system.
6. Determination of pK_a of indicators by colorimetry.
7. Evaluation of rate constant of first order reaction by potentiometry.
8. Colorimetric estimation of aspirin.
9. Determination of the Fe by colorimetry.
10. Determination of Cu by colorimetry.
11. Experiment to be designed by students.

REFERENCES

1. Findlay's Practical Physical Chemistry, revised by Levitt, Longman's, London (1966).
2. Experiments in Physical Chemistry, Shoemaker and Garland, McGraw Hill International edition. (1996).
3. Advanced Practical Physical Chemistry, J B Yadav, Goel Publication House, Meerut.
4. Experimental Physical Chemistry, Daniel et al.,McGraw Hill (1962).

Semester	II
Paper Code	CH8P2
Paper Title	PHYSICAL CHEMISTRY PRACTICAL II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

Physical Chemistry Practical II

1. Titration of a mixture of strong and weak acids/bases and salt against a strong base/acid by conductometric method.
2. Estimation of urea by enzyme hydrolysis using conductance method
3. Determination of dissociation constant of a weak acid or weak base by conductometry.
4. Determination of Onsagar parameters for a strong electrolyte by conductometry.
5. Determination of thermodynamic parameters of micellization of a surfactant from conductivity measurements.
6. Potentiometric estimation of extent of intercalation.
7. Titration of a weak acid against a strong base using quinhydrone electrode and calculation of pKa values of the weak acid.
8. Titration of a mixture of strong and weak acids potentiometrically and the determination of the composition of the mixture.
9. Determination of activity coefficient of H^+ by potentiometry.
10. Degree of hydrolysis of aniline hydrochloride by potentiometry.
11. Experiment to be designed by students.

REFERENCES

1. Findlay's Practical Physical Chemistry, revised by Levitt, Longman's, London (1966).
2. Experiments in Physical Chemistry, Shoemaker and Garland, McGraw Hill International edition. (1996).
3. Advanced Practical Physical Chemistry, J B Yadav, Goel Publication House, Meerut.
4. Experimental Physical Chemistry, Daniel et al.,McGraw Hill (1962).

Semester	II
Paper Code	CH8P3
Paper Title	Synthesis and Characterization of Compounds I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

Inorganic Compounds:

1. Preparation and quantitative analysis of hexamminecobalt (III) chloride.
2. Preparation of potassium trioxalatoferrate (III) trihydrate and its characterization by quantitative analysis and IR studies.
3. Preparation of a variety of complexes (5 Nos.) and their characterization by UV-Visible and IR techniques.
4. Preparation of a nano materials and their characterization by UV spectroscopy (band gap) and XRD (crystallite size).
5. Synthesis of spinels and its characterization by XRD studies.

REFERENCES

1. Handbook of Preparative Inorganic Chemistry, G Brauer, Academic Press (1963).
2. Practical Inorganic Chemistry, Marr and Rocket
3. Laboratory Manual of Organic Chemistry, Day, Sitaraman and Govindachari (1996).
4. Practical Organic Chemistry, Mann and Saunders (1980).
5. Textbook of Practical Organic Chemistry, A I Vogel (1996)
6. A Handbook of Organic Analysis, Clarke and Hayes (1964).

Semester	II
Paper Code	CH8P4
Paper Title	Synthesis and Characterization of Compounds II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

Organic Compounds:

1. Preparation of benzanilide from benzophenone.
2. Preparation of benzilic acid from benzoin.
3. Preparation of anthranilic acid from phthalic acid.
4. Preparation of 2-iodoxy benzoic acid (IBX) from anthranilic acid and its application for the oxidation of alcohol.
5. Preparation of dibenzalacetone and reduction of carbonyl group.
6. Application of *N*-bromosuccinimide (NBS) in allylic bromination.
7. Preparation of an organic compound (one step preparation) by 2 or 3 different methods and comparison/evaluation of the methods with respect to the following parameters:

(i) Ease of preparation, problems in handling chemicals, toxicity and flammability of chemicals

(ii) Yield and cost effectiveness

(iii) Product purity/quality

(iv) Environmental compatibility (from the point of view of green chemistry)

8. Any other experiments

Characterization of the organic compounds (experiments 8–14) by: TLC, column liquid chromatography, fractional crystallization, UV, IR and NMR spectroscopic techniques.

REFERENCES

1. Handbook of Preparative Inorganic Chemistry, G Brauer, Academic Press (1963).

2. Practical Inorganic Chemistry, Marr and Rocket

3. Laboratory Manual of Organic Chemistry, Day, Sitaraman and Govindachari (1996).

4. Practical Organic Chemistry, Mann and Saunders (1980).

5. Textbook of Practical Organic Chemistry, A I Vogel (1996)

6. A Handbook of Organic Analysis, Clarke and Hayes (1964).

THIRD SEMESTER
THEORY PAPERS

Semester	**III**
Paper code	**OCH9122**
Paper title	**ORGANIC SYNTHESIS-I**
Number of teaching hrs per week	**04**
Total number of teaching hrs per semester	**60**
Number of credits	**04**

1. Important reactions in organic synthesis (7+1) h

C-C bond formation: Henry, Peterson's olefination, Bamford-Stevens, McMurry coupling, Robinson Annulation, Stobbe reaction, Darzen's reaction, Horner-Wadsworth-Emmons, Shapiro reaction.

C-O bond formation: Stork-enamine synthesis, Acyloin condensation.

C-N bond formation: Barton reaction, Mannich reaction

Wittig reaction, Perkin reaction, Dieckmann condensation, Claisen ester condensation, Knoevenagel condensation.

2. Oxidation-reduction reactions in organic synthesis (11+2) h

Applications of peroxides (hydrogen peroxide, *t*-butyl peroxide, dibenzoylperoxide), peracids (CF_3COOOH, m-CPBA, monoperphthalic acid) as oxidizing agents, HIO_4, lead acetate, DDQ, Selenium dioxide, Chromium (VI) and Manganese (VII) as oxidants. Dess-Martin oxidation, Sharpless asymmetric epoxidation and Oppanaeur oxidation.

Complex metal hydrides, diimide reduction, organoboranes, LDA, trimethylsilyl iodide, Woodward and Prevost reagent, NBS, Benkeser reduction, Wolf-Kishner reduction, Meerwin-Pondorff Verley reduction, Pummer, Willgredot, Corey-Bakshi-Shibata reaction and Tischenko reaction.

Applications of Ozone and Osmium tetroxide as oxidants, Birch and Clemmenson reduction.

3. Organometallics in organic synthesis (8+1 h)

Organolithium compounds - application in deprotonation of C-H bonds, ortho directing effect, addition to multiple bonds (anionic polymerization), lithium-halogen exchange, synthesis of organometallics (via transmetalation). Organomagnesium compounds (Grignard reagent), application in organometallic synthesis, application of organozinc compounds (ZnR_2) in

Simmons-Smith reaction, Gilman reagent mediated organic synthesis using Me_2CuLi as an example.

Organomagnesium compounds (Grignard reagent), application in organic synthesis

4. Transition metal complexes (homogeneous catalysis) in organic synthesis (12+3 h)

Catalytic cycle and key reaction steps in homogeneous catalysis-ligand dissociation, association, oxidative addition-reductive elimination, substrate coordination, insertion/de-insertion, transmetalation, nucleophilic attack on substrate.

Catalytic hydrogenation (catalytic cycle of Wilkinson Catalyst), Asymmetric hydrogenation including transfer hydrogenation (Noyori catalyst with mechanism).

Alkene metathesis reactions-mechanism, Schrock catalyst, Grubbs catalysts (I and II generation)

Metal catalyzed coupling reactions: Pd catalyzed cross-coupling reactions, mechanism of overall cross coupling reactions, effect of catalyst structure on cross coupling reactions (effect of chelation, effect of steric properties, ligand electronic properties), substrate scope, reaction conditions(catalytic precursors, phosphine and N-heterocyclic carbene ligands), Mizoroki-Heck reaction (catalytic cycle with examples), application of Suzuki, Negishi, Kumada, Hiyama, Stille reactions, Tsuji-Trost (mechanism) and Buchwald-Hartwig reactions (catalytic cycle with examples). Copper catalyzed C-C and C-heteroatom bond forming reactions.

18- and 16-electron rules. Current trends in homogeneous catalysts.

Problem Solving: ***Problems based on 18- and 16-electron rules***

5. C-H bond activation in organic synthesis 5h

Introduction: Importance of C-H activation, types of C-H bond activation, green chemistry involved in C-H activation.

Mechanism of different types of C-H activation: radical-mediated, metal mediated (homolytic, heterolytic and σ-bond metathesis pathways). Example: Palladium catalyzed C-H bond activation reactions.

Chelation assisted functionalization of arenes, borylation of arenes, hydroacylation of alkenes, alkynes.

C-H bond activation of heteroaromatics, metal-catalyzed oxidation of C-H bond to C-N bond.

6. Heterogeneous catalysis in organic synthesis (4+1h)

Introduction, difference between homogeneous and heterogeneous catalyst, characteristics of heterogeneous catalysts, active sites in catalysts

Solid acid/base and oxidation catalysts: heteropolyacids (keggin structure, $H_4SiW_{12}O_{40}$ - toluene alkylation), clays (montmorollite K-10, acylation), ion exchange resins- (esterification reaction), MgO (aldol condensation) V_2O_5/Al_2O_3 (synthesis of nicotinic acid)

Zeolites: pore size and channel variation with Si/Al ratio, shape selectivity, reactant and product selectivity; e.g. - para xylene synthesis).

Heterogenising aspects of homogeneous transition metal complexes: Immobilization of transition metal complex catalysts on supports, catalyst deactivation pathways-leaching mechanism.

7. Introduction to electro-organic synthesis (5h)

Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes. Cell design-Undivided, quasi-divided and divided cell. Modes of operation-Galvanostatic and potentiostatic. (3h)

Anodic oxidation: Kolbe reaction, Shono oxidation, selective C-H activation reactions (arylation) (1h).

Cathodic reduction: Reduction of alkyl halides, nitro compounds and arenes (1h).

REFERENCES:

1. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry. Part B: Reactions and Synthesis. 5^{th} edition, Springer publishers, 2007.
2. M. B. Smith, Organic Synthesis 4^{th} Edition, Elsevier Inc. 2017.
3. W. Carruthers and L. Coldham. Modern Methods of Organic Synthesis, 4^{th} edition, Cambridge University Press, 2004.
4. J. Clayden, N. Greeves and S. Warren, Organic Chemistry, Oxford University Press, 2012
5. J. F. Hartwig, Organotransition Metal chemistry, University Science Books, 2010.
6. A. J. Elias, B. D. Gupta, Basic Organometallic Chemistry 2^{nd} Edition, Universities Press, 2013.
7. M. Bochmann, Organometallics and Catalysis, Oxford University Press, 2015
8. C. Elschenbroich, Organometallics 3^{rd} Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2006.
9. R. H. Crabtree, The Organometallic Chemistry of Transition Metals, 6^{th} edition, John Wiley & Sons 2014.
10. Metal-Catalyzed Cross-Coupling Reactions and More, 2^{nd} Edition. Editors: A. de Meijere, S Bräse, M Oestreich, Wiley-VCH Verlag GmbH & Co., Weinheim, Germany, 2014.
11. C-H bond activation in organic synthesis. Editor: J. J. Li., CRC Press, 2017.
12. Applied Homogeneous Catalysis with Organometallic Compounds 3^{rd} Edition. Editors: B. Cornils, W Hermann, M Beller and R Paciello, Wiley-VCH Verlag GmbH & Co., Weinheim, Germany, 2018.
13. O. Hammerich and B. Speiser, Organic electrochemistry, 5^{th} edition, CRC Press, 2016.

14. T. Fuchigami, M. Atobe and S. Inagi, Fundamentals and Applications of Organic Electrochemistry, John Wiley & Sons 2015.
15. "Electro-organic synthesis – a 21st century technique", D. Pollok and S. R. Waldvogel, *Chem. Sci*. **2020**, *11*, 12386–12400.
16. "The Shono-type electroorganic oxidation of unfunctionalized amides. Carbon–carbon bond formation via electrogenerated *N*-acyliminium ions", A. M. Jones and C. E. Banks, *Beilstein J. Org. Chem.* **2014**, *10*, 3056–3072.
17. Modern Heterogeneous Catalysis, an Introduction by R. A. van Santen, Wiley VCH, 2017-1, 54.
18. V. S. Gerard, N. Ferenc, Heterogeneous Catalysis in Organic Chemistry; Academic Press; New York. 1st ed, 2006.
19. M. Benaglia, A. Puglisi, Catalyst Immobilization, Wiley-VCH Verlag GmbH & Co. 2020.
20. R. L. Augustine, Heterogeneous Catalysis for the Synthetic Chemist, New York, CRC Press, 1996.
21. D. K. Chakrabarty, B. Viswanathan, Heterogeneous Catalysis, New Age Science. 2009.

Semester	III
Paper Code	OCH9222
Paper title	**ORGANIC SYNTHESIS - II**
Number of teaching hours per week	3
Total number of teaching hours per semester	45
Number of credits	3

RETROSYNTHESIS **(27 + 3) h**

i) Disconnection approach:

Basic principles; introduction to synthons and synthetic equivalents.

Latent polarity, Functional group interconversion. *Oxidizing and reducing agents*.

Synthesis of aromatic compounds, order of events.

One-group C-X and two-group C-X disconnections.

Reversal of polarity (Umpolung), synthesis of cyclic compounds; amine synthesis.

Protecting groups; Protection of alcohols, ***carbonyl compounds***, amines and carboxylic acids.

One group C-C disconnections.

Chemoselectivity, alkene synthesis, use of acetylides.

Two group C-C disconnections: ***Diels-Alder reactions***; 1,3-, and 1,5-, difunctionalized compounds, α, β-unsaturated carbonyl compounds, carbonyl condensations, Michael addition and Robinson annulation. Use of aliphatic nitro compounds.

Introduction to ring synthesis: synthesis of 3,4,5,6 membered rings and saturated heterocycles

ii) Strategy and planning a synthesis-convergent and linear synthesis.

Convergent synthesis: differences between convergent and linear synthesis. Advantage of convergent synthesis over linear synthesis

Convergent synthetic strategy for ferruginol, α-bisabolene.

Failure of convergent synthesis with multistriatin as example. Linear synthesis of multistriatin. Combination of linear and convergent synthesis, starting material and key aspects of reaction. Industrial synthesis of α- and β-sinensals as examples for the above.

2. REVIEW ARTICLE BASED MODERN ASPECTS OF ORGANIC CHEMISTRY
(12 + 3) h

REFERENCES:

1. Organic Synthesis: The Disconnection Approach by Stuart Warren (Wiley India)
2. Workbook for Organic Synthesis - The Disconnection Approach by Stuart Warren (John Wiley, 1983)

3. Organic Synthesis by Christine Wills and Martin Wills (Oxford University Press, 2005)
4. Organic Synthesis - Design, Reagents, Reactions and Rearrangements by Jagadamba Singh and D.S.Yadav (Pragati Prakashan, 2007)
5. Principles of Organic Synthesis by R.O.C Norman and J.M Coxon (Chapman and Hall)
6. Advanced Organic Chemistry by Carey and Sundberg part B, 5^{th} Edn.

Semester	III
Paper Code	OCH9322
Paper title	CHEMISTRY OF HETEROCYCLIC COMPOUNDS, BIOMOLECULES AND NATURAL PRODUCTS
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

1. HETEROCYCLIC CHEMISTRY (20+2)h

Five-membered heterocycles with one heteroatom: pyrrole, furan and thiophene- aromaticity and reactivity order, resonance, synthesis and chemical reactivity.

Six- membered heterocycles with one heteroatom: basicity, synthesis and chemical reactions of quinoline, isoquinoline, indole.

Azoles: synthesis and chemical reactions of 1,2,3-triazole and 1,3,4-oxadiazole.

Azines: diazines (pyridazine, pyrimidine, pyrazine) and triazines (1,2,3-triazine, 1,2,4-triazine & 1,3,5-triazine).

Benzo-fused heterocycles: synthesis and reactions of benzofurans, benzothiophenes, benzoxazoles and benzothiazoles.

Three and four membered oxygen and nitrogen containing heterocycles- name and structure.

2. PEPTIDE CHEMISTRY (2h)

Introduction to peptides. Synthesis of peptides: chemical and Merrifield synthesis.

3. CARBOHYDRATES (5+1)h

Classification, structure and general properties of carbohydrates. Structure and functions of polysaccharides and complex carbohydrates; amino sugars, proteoglycans and glycoproteins.

4. TERPENES (9+1)h

Structural elucidation, biosynthesis and synthesis of α-pinene (an example of bicyclic monoterpene), farnesol (an example of acyclic sesquiterpene) and abietic acid (an example of tricyclic diterpene). Commercial synthesis of camphor.

Carotenoids: Methods of isolation, structural relationship of α -, β- and γ- carotenes. Structure elucidation, biosynthesis and synthesis of β-Carotene. Conversion of β-carotene to Vitamin A.
Classification, nomenclature, occurrence, isolation of terpenes. Isoprene rule, stereochemistry of citral, limonene, menthol and borneols.

5. ALKALOIDS (6+1)h
Structural elucidation, biosynthesis and synthesis of Quinine (an example of quinoline alkaloid), Morphine (an example of opiate alkaloid) and reserpine (an example of indole alkaloid).
Definition, nomenclature, occurrence and classification of alkaloids.

6. CHEMISTRY OF VITAMINS 4h
Structural elucidation, biosynthesis and synthesis of haemin and Vitamin B_{12} (synthesis of Vitamin B_{12} from cobyric acid).

7. INSECT PHEROMONES (2+1) h
Introduction and classification. Stereoselective synthesis of bombykol and 3,11-dimethyl-2-nonacosanone.
Pheromones in pest control.

8. PROSTAGLANDINS 6h
Introduction, nomenclature, classification and biological role of prostaglandins. Biosynthesis of prostaglandins, conversion of arachidonic acid to prostaglandins, prostacyclins and thromboxanes. Structural elucidation and stereochemistry of PGE1. Synthesis of PGE1 by Corey's approach. Synthesis of PGE2 by Upjohn's approach. Synthesis of prostacyclin I2 and Thromboxane B2.

REFERENCES:
1. S. P. Bhutani. Organic Chemistry: Selected topics. 2008, Ane Books.
2. J. A. Joule, K. Mills, G. F. Smith. Heterocyclic Chemistry. 5th edition, 2010. John Wiley and sons Ltd.
3. R. M. Acheson. An introduction to Heterocyclic Chemistry. 3rd edition, 2008. Wiley India Pvt. Ltd.
4. Raj. K. Bansal. Heterocyclic Chemistry. 5th Edition, 2017. New Age International publishers.
5. S. P. Bhutani. Chemistry of Biomolecules: Selected topics. 2008, Ane Books.

6. Chemistry of natural products, Kalsi, Kalyani Publishers, 1983.
7. Chemical Aspects of Biosynthesis, J. Mann, Oxford Science Publications, 1994.
8. Natural products: Their Chemistry and Biological Significance, J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe and J. B. Harborne (Longman, UK,1994).
9. Terpenes, J. Verghese (Tata Mc graw-Hill, New Delhi, 1982).
10. Chemistry of terpenes and terpenoids, A. Newman (Academic press, London,1975).
11. Organic Chemistry by I. L. Finar, vol II, (6thEdn, Longman, 1992).
12. Chemistry of natural products vol I and II by O.P. Aggarwal (Goel Publishing house, 6^{th} edn,1982).
13. The Colours of Life: An Introduction to the Chemistry of Porphyrins and Related Compounds by L.R. Milgrom (Wliey Chichester, 1995).
14. Organic Chemistry of Natural products Vol I and II by Gurudeep R. Chatwal, ed: M. Arora (Himalaya publishing House, New Delhi, 2015).
15. Chemistry of Natural Products: A Unified Approach by N.R. Krishnaswamy (University press, London, 1999).
16. Total Synthesis of Natural products: The Chiral Approach, Vol III by S. Hanessian (Pergamon Press, 1983).
17. Medicinal Natural products: A Biosynthetic Approach by P.M. Dewick (John Wiley, Chichester,1997).

Semester	III
Paper code	OCH9422
Paper title	STEREOCHEMISTRY AND ASYMMETRIC SYNTHESIS
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

1. STEREOCHEMISTRY OF UNSATURATED ACYCLIC, FUSED, BRIDGED AND CAGED SYSTEMS 14 h

(*Recall: Stereochemistry of fused rings and bridged rings*).

Stereochemistry of fused, bridged and caged systems: paddlanes and propellanes; catenanes, rotaxanes, knots, and Möbius strips; cubane, tetrahedrane, dodecahedrane, adamantane and buckminsterfullerene

Conformations of unsaturated acyclic and miscellaneous compounds.

2. EFFECT OF CONFORMATION ON REACTIVITY 8 h

Diastereomer equilibria in acyclic systems.

Conformation and reactivity: the Winstein-Holness equation and the Curtin-Hammett Principle.

3. ASYMMETRIC SYNTHESIS (15+2) h

'Enantiomeric excess' (*ee*) and methods of determination of '*ee*'. Stereoselectivity: classification, terminology and principle. Asymmetric synthesis and asymmetric induction. Double diastereoselection and double asymmetric induction.

Acyclic stereoselection: Addition of nucleophiles to carbonyl compounds (1,2- 1,3- and 1,4-asymmetric induction). Asymmetric aldol condensation, Zimmerman-Traxler model. Addition of allylmetal and allylboranes to carbonyl group.

Diastereoselection in cyclic systems: Nucleophilic addition to cyclic ketones (formation of axial and equatorial alcohols, exo-endo selection), catalytic hydrogenation (haptophilic stereocontrol), alkylation (α-alkylation of (*S*)-proline), diastereoselective oxidations, enantioselection of OsO_4 dihydroxylation using chiral diamines, stereoselective cyclization of polyenes (biomimetic synthesis of progesterone) .

Enantioselective synthesis: Reduction with chiral hydride donors [(*S*)-PBMgCl,(-)-iBOAlCl_2, alpineborane, (*S*)-BINAL-H, (*R*,*R*)-DIOP, (*S*,*S*)-CHIRAPHOS].

Enantioselective alkylation of ketones via hydrazones (SAMP, RAMP). Enantioselective alkylation with chiral PTC. Enantioselective Michael addition. Enantioselective intramolecular aldol condensation and Robinson annulation. Use of (+)- and (–)- DET in Sharpless asymmetric epoxidation. Asymmetric amplification.

***Polymer-bound chiral catalysts in asymmetric induction*.**

4. CHIRAL RESOLUTION TECHNIQUES (7+1) h

Separation of enantiomers via crystallization (conglomerates); chemical separation of enantiomers via diastereomers: introduction to resolving agents, resolving agents for a few functional groups (acids, lactones, bases, aldehydes, ketones and amino acids).

Diastereomers: Asymmetric transformations, general methods of separation, chromatographic resolution.

Enantiomeric enrichment as a resolution strategy in nonracemic samples.

Large scale resolution: diastereomer mediated resolution, resolution by preferential crystallization, kinetic resolution, enzymatic resolution.

chiral chromatography for enantiomeric resolution

5. CHIROPTICAL PROPERTIES (11+2) h

Meaning of chiroptical properties; optical activity, anisotropic refraction: theory, optical rotatory dispersion (ORD).

Circular dichroism (CD), anisotropic absorption.

Applications of ORD and CD: Determination of configuration and conformation (theory); classification of chromophores; sector and helicity rules: α-axial haloketone rule, Octant rule, Benzene quadrant rule, Snatzke's Benzene sector rule, Lowe's rule for allenes; exciton chirality rule or dibenzoate chirality rule. Correlation of Optical rotation and group polarizability: Brewster's rule. Effect of solvent polarity on CD of (-)menthone.

Other applications: induced ORD and CD; fluorescence detected circular dichroism; circular dichroism of chiral polymers. Vibration optical activity. Circular polarization of emission; anisotropic emission.

REFERENCES

1. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley and Sons, 2016.

2. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2nd Edn., New Age International Publishers, 2001.

3. Stereochemistry: Conformation and Mechanism, P.S. Kalsi, 10^{th} Edn., New Age International Publishers, 2019.

4. Organic chemistry Volume 2: Stereochemistry and the Chemistry of Natural products, I. L. Finar, 5th Edn, Longman Singapore Publishers Pte Ltd, 1975
5. Circular Dichroism: Principles and Applications, N. Berova, K. Nakanishi, R. W. Woody, 2nd Edn., John Wiley & Sons Inc., 2000.
6. Chiroptical spectroscopy: Fundamentals and applications, 1st Edn., Prasad L. Polavarapu, CRC Press, Taylor & Francis Group, 2017.

Semester	III
Paper code	CHOE 9521
Paper title	Open elective: LIFE'S LABORATORIES
Number of teaching hours per week	2
Total number of teaching hours per semester	30
Number of credits	2

1. CHEMISTRY AND SOCIETY **2 h**

An introduction of the impact of chemistry on society.

2. MOLECULAR GASTRONOMY **5 h**

Introduction to molecular gastronomy: history & development. Chemical structures and properties of food; colloid chemistry; emulsions culinary/cooking processes: freezing, heating (conduction, convection, radiation); applications. A preliminary knowledge of flavors, colors, emulsifiers stabilizers, additives. Novel ingredients and delivery mechanisms. Laboratory based technologies (including water baths, freeze drying).

3. FORENSIC CHEMISTRY **5 h**

What is forensic science? An idea of the analytical techniques used: a) Atomic Spectroscopy b) Microspectrophotometry c) Electrophoresis d) Microscopy e) Chromatography f) Immunoassays. Analysis of forensic samples – a) Drug analysis b) Combustion & arson c) Inks, paints, & pigments d) Polymers & fibers

4. MOLECULAR PROCESSES **3 h**

Biological clock, circadian clock; Molecules involved and their interactions. Consequences of sleep deprivation – physiological and neurological – molecules and their interplay.

5. GREEN CHEMISTRY AND THE INDUSTRY **5 h**

What is green chemistry? What are the current chemical industries?
What are green processes?

6. RESEARCH BASED PEDAGOGY TOOLS **10 h**

Relate your master’s subject with chemistry – this involves reading, presentation and design of an experiment (wet or dry lab) that can be demonstrated.

REFERENCES:

1. Chemistry: Impact On Society:- Melwin D. Joesten, David O Johnston, John T. Netterville and James L. Wood, Saunders Golden Sunburst Series; Saunders College Publishing.
2. The ESSENCE Of GASTRONOMY Understanding the Flavor of Foods and Beverages, Peter Klosse CRC PressTaylor & Francis Group International Standard Book Number-13: 978-1-4822-1677-6 (eBook - PDF), 2013.
3. Biochemistry - Gareth and Grisham, Saunders College Publishing.
4. New trends in green chemistry - Ahluwalia and Kidwai, Anamaya Publishers, 2004.
5. Forensic Chemistry - Suzanne Bell - Pearson Publishers, 2012.

Semester	III
Paper code	CHOE 9622
Paper title	Open elective: **Culinary Chemistry**
Number of teaching hours per week	2
Total number of teaching hours per semester	30
Number of credits	2

1. SCIENCE IN THE HOME KITCHEN **6 hrs**

The variability challenge - ingredient variables, equipment variables, technique variables; The modes of learning how to cook (expert instruction, observation, trial & error, question and answer).

Three ways of starting a chemical reaction in kitchen:

(i) knives **(**mechanical force) as a catalyst for chemical change. **Case study**: Reason for sweet oranges sometimes resulting in bitter juice; reason for sliced onions making people cry; blanched basil leaves

(ii) Heat - Chemicals that give fruits and plants their colour: chlorophyll, carotenoids and anthocyanins. Effect of cooking and pH on colour of fruits and vegetables, effect of heat on fruits and vegetables.

(iii) Combination of Ingredients **-** the anatomy of meat, tenderizing of meat, the science of marinating. **Case study**: The curious case of the shrinking apple pie. Eggs : It's All about foams and coagulation - the science of whipping, heat and role of fat in coagulation ; testing the tenderness of Eggs (cooked with and without butter).

2. METHODS OF COOKING **5 hrs**

Cooking media – air, water, steam and fat, microwave cooking – method, advantage & disadvantages, techniques of cooking - roasting, baking, frying, boiling, steaming, grilling etc.

3. CHEMISTRY OF COOKING **7 hrs**

Food additives/taste modifiers: salt, sugar, baking soda, baking powder, sour powder, cream of tartar, vanilla extract, MSG (monosodium glutamate), colorants and antioxidant agents. Chemicals produced while cooking and their harmful effects: polyaromatic hydrocarbons, nitrosamines, saturated fats.

4. GRAINS, BREAD AND LEAVENING 7 hrs

The basic structure of dough, batter and their products: gluten, starch, gas bubbles, fats; comparison of yeasts and chemical leavenings. Mailard reaction, science behind the production of bread: ingredients, mixing and kneading, fermentation, baking and the role of steam; how to improve dough: investigation of protein bonds that form its glutinous network.

Activity: Demonstration of dough-making for muffins, brownies and cakes.

5. AMATEUR TO FOOD SCIENTIST 5 hrs

The science involved in making biriyani, brownies, chocolate chip cookies, French fries, hamburgers, ice cream sundaes, omelette, pancakes and pudding.

References

1. ‘On food and Cooking, the science and lore of the kitchen’, Harold McGee, Ed. Scribner, Chapter 10 pp 521-571.

2. ‘Kitchen science explained, what Einstein told his cook’, Robert L. Wolke, Ed. W.W. Norton and company, chapter 3, pp 97-109 and 114-116 .

3. Developments in Dairy Chemistry. Fox, P. F. (Ed). (1982). Applied Sci. Publ., NewYork.

4. Fox, P. F. and Sweeny, Mc. (1998). Dairy Chemistry and Bio-Chemistry. Academic Platinum Publ., New York.

5. Fox, P. F. (Ed). (2006). Developments in Dairy Chemistry. Applied Sci. Publ., NewYork.

6. Jenness, R. and Patton, S. (1984). Principles of Dairy Chemistry. Wiley Eastern Pvt. Ltd, New Delhi.

7. Mathur, M. P., Datta, D. R., and Dinakar, P. (1999). Text book of Dairy Chemistry, Directorate of Information and Publs., ICAR, New Delhi.

8. Webb, B. H., Johonson, A. H., and Alford, J. A. (Eds). (2008). Fundamentals of Dairy Chemistry. CBS Publ. and Distributors Pvt. Ltd., New Delhi.

THIRD SEMESTER
PRACTICAL PAPERS

Semester	III
Paper Code	OCH9P1
Paper Title	PRACTICAL : SEPARATION AND IDENTIFICATION OF ORGANIC COMPOUNDS
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

This practical course involves purification and analysis of a mixture of organic compounds. The components of the given mixture would be purified by recrystallization, solubility and distillation techniques, TLC, column chromatography, HPLC followed by spectroscopic characterization. Application of advanced qualitative analysis: Preparation and characterization of organic compounds having *o*- and *p*- isomers (separation of isomers from crude products) (11 sessions).

1. Purification of mixture of organic compounds by recrystallisation.
2. Identification and separation of mixture of organic compounds using TLC.
3. Separation of mixture of organic liquid compounds using distillation.
4. Separation of mixture of organic compounds using column chromatography.
5. Separation of mixture of organic compounds using HPLC.
6. Separation of mixture of organic compounds using solubility techniques and their structure elucidation using FT-IR and UV-vis spectroscopic techniques.
7. Separation of mixture of organic liquid compounds using distillation and their characterisation using spectroscopic techniques.
8. Separation of mixture of organic compounds using column chromatography and their structural characterisation using spectroscopic techniques.
9. Synthesis of an organic compound giving isomers (Need to select specific synthesis).

10. Identification of isomers of synthesized organic compound using TLC, purification using column chromatography and structural characterisation using spectroscopic techniques (2 sessions).

11. Any other related experiments based on the syllabus (e.g., experiments on polarimeter).

REFERENCES

1. Vogel's Textbook of Quantitative Chemical Analysis, 5th edition, G N Jeffery, J Bassett, J Mendham and R C Denny, Longman Scientific and Technical (1999).
2. Practical organic chemistry, A. K. Manna, Books and Allied (P) Ltd, 2018.
3. An Advanced course in practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, New Central Book Agency (P) Ltd, 2nd edition reprinted 2018.

Semester	III
Paper Code	OCH9P2
Paper Title	ORGANIC SYNTHESIS- I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

This practical course involves single-step and two-step organic synthesis, characterization of the products through relatively simple techniques like thin layer chromatography and melting point determination. It also includes UV/IR spectral analysis of the products.

One-stage synthesis:

1. Synthesis of adipic acid from cyclohexanol
2. Synthesis of tetrahydrocarbazole from cyclohexanone and phenylhydrazine by Fischer indole synthesis

Two-stage synthesis:

3. Synthesis of 2,5-hydroxyacetophenone starting from resorcinol and acetic acid (Fries rearrangement)
4. Synthesis of an α, β- unsaturated acid starting from anisaldehyde (Knoevenagel condensation)
5. Synthesis of polyhaloarene (1-iodo-2,4,6-tribromoaniline) starting from aniline
6. Synthesis of trimethylquinoline from p-toluidine (Paal Knorr synthesis)

REFERENCES

1. Vogel's Textbook of Quantitative Chemical Analysis, 5^{th} edition, G N Jeffery, J Bassett, J Mendham and R C Denny, Longman Scientific and Technical (1999).

2. Practical organic chemistry, A. K. Manna, Books and Allied (P) Ltd, 2018.

3. An Advanced course in practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, New Central Book Agency (P) Ltd, 2^{nd} edition reprinted 2018.

Semester	III
Paper Code	OCH9P3
Paper Title	PRACTICAL: ORGANIC SYNTHESIS-II
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

This practical course involves slightly advanced organic synthesis meant to train students for higher academic/ industrial research, purification of the synthesized compounds, characterizations through simple techniques like thin layer chromatography and melting point analysis, and advanced instrumental characterization of the purified compounds. It also includes the spectral analysis of the compounds.

Organic Synthesis, purification, characterization 11 sessions

1. Preparation of dry solvents (1 session)
2. Protection and selective deprotection of functional groups (2 sessions)
3. Azidation using crown ethers (selective protection of primary alcohol) (2 sessions)
4. Dicyclohexylcarbodiimide (DCC) mediated coupling reaction (1 session)
5. Grignard reaction (3 sessions)
6. Wittig reaction (2 sessions)

REFERENCES

1. Practical organic chemistry, A. K. Manna, Books and Allied (P) Ltd, 2018.
2. An Advanced course in practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, New Central Book Agency (P) Ltd, 2nd edition reprinted 2018.

Semester	III
Paper Code	OCH9P4
Paper Title	PRACTICAL: ORGANIC SYNTHESIS-III
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Organic Synthesis, purification, characterization (11 sessions)

This practical course involves comparatively greener methods of organic synthesis meant to train students for higher academic/ industrial research, purification of the synthesized compounds, characterizations through simple techniques like thin layer chromatography and melting point analysis, and advanced instrumental characterization of the purified compounds. It also includes the spectral analysis of the compounds.

Organic Synthesis, purification, characterization

1. Conversion of Benzhydrol to Benzophenone by different oxidation reactions and to assess the green chemistry index. (2 sessions)
2. Solvent-free reductive amination using mortar and pestle (2 sessions)
3. Proline catalyzed reaction in water (2 sessions)
4. Suzuki coupling in pure water (2 sessions)
5. Photoxidation of alcohol with heterogeneous photocatalysts in the UV range (1 session)
6. 1,4-Cyclohexadiene with Pd/C as a rapid, safe transfer hydrogenation system with microwave heating. (1 session)
7. Microwave assisted nitration of phenol using copper nitrate. (1 session)
8. Evaluation of the Photocatalytic degradation of Benzoquinone/2-chlorophenol in the aqueous phase using ZnO and TiO_2 Photocatalysts. (1 session)
9. Synthesis and Evaluation of biodiesel from waste vegetable oil (2 sessions)

REFERENCES

1. Practical organic chemistry, A. K. Manna, Books and Allied (P) Ltd, 2018.

2. An Advanced course in practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, New Central Book Agency (P) Ltd, 2nd edition reprinted 2018.

FOURTH SEMESTER
THEORY PAPERS

Semester	IV
Paper Code	OCH0221
Paper Title	Medicinal Chemistry
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

1. MOLECULAR ASPECTS OF DRUG ACTION (10 + 2) h

Drug, API, drug additives (brief account of classification and meaning of different additives), Difference between drugs and medicines. Drug targets, receptors, receptor types, drug- receptor interaction (forces involved), agonist, antagonist, partial agonist (dose response curves), drug synergism, drug resistance, physicochemical factors influencing drug action, pharmacokinetics, pharmacodynamics, isosterism and bioisosterism, theories of drug –receptor interaction. Assay of drugs: Chemical assay, biological assay, immunological assay, ***LD_{50}, ED_{50}, IC_{50}, ID50 and EC_{50}. Metal ion toxicity and detoxification - chelation therapy***

2. CLASSIFICATION OF DRUGS BASED ON THERAPEUTIC ACTION (24 + 4) h

Antibiotics: Introduction, targets of antibiotics action, classification of antibiotics, mechanism of action of penicillin, cephalosporin, β-lactamase inhibitors, tetracyclines, aminoglycoside and macrolides. Synthesis of penicillin.

Antivirals: Neuraminidase inhibitors (oseltamivir phosphate as an example), inhibitors of viral replication (acyclovir as an example), reverse transcriptase inhibitors (zidovudine and abacavir as examples). Synthesis of acyclovir.

Analgesics, antipyretics and anti-inflammatory Drugs: mechanism of inflammation, ***classification and mechanism of action of NSAID*** (aspirin, paracetamol and ibuprofen as examples). ***Synthesis of ibuprofen***.

Antihistamines: Mode of action of H1 and H2 antihistamines (chlorpheniramine, cetirizine and ranitidine as examples).

Antidiabetics: types of diabetics, types of drugs used for the treatment and their mode of action (sulfonylureas, α-glucosidase inhibitors, biguanides, dipeptidyl peptidase-4 (DPP-4) inhibitors, Glucagon-like peptide-1 receptor agonists (GLP-1 receptor agonists), meglitinides, sodium-glucose transporter (SGLT) 2 inhibitors, sulfonylureas, thiazolidinediones). Synthesis of metformin.

Cardiovascular drugs: cardiovascular diseases, different classes of drugs acting on the cardiovascular system such as antianginal drugs, antiarrhythmic agents and antihypertensive agents.

Anti-neoplastic agents: Introduction, drug classes: alkylating agents- organoplatinum compounds, antimetabolites - purine, pyrimidine and folate drugs, antibiotics- actinomycins and anthracyclins, kinase inhibitors, natural products- mitotic inhibitors.

Central Nervous System (CNS) drugs: CNS depressants- anxiolytics, sedatives, hypnotics, antipsychotics. CNS stimulants- anti-depressants.

3. STAGES OF DRUG DEVELOPMENT AND DRUG DISCOVERY (11 + 1) h

Procedure followed in drug design: drug discovery with and without a lead. Lead discovery.

Lead modification: Drug design and development, ADME, identification of active part: pharmacophore, functional group modification, structure-activity relationship (SAR). Structure modification to increase potency and the therapeutic index: homologation, chain branching, ring-chain transformation, bioisosteric structural modification to increase oral bioactivity (electronic effect, the Hammet equation & lipophilicity effect), peptidomimetics, Combinatorial chemistry.

Preclinical toxicology testing and IND application: regulatory acts and regulatory bodies, main stages of preclinical toxicology testing-acute toxicity studies, repeated dose studies, genetic toxicity studies, reproductive toxicity studies, carcinogenicity studies and toxicokinetic studies.

Clinical trials: Phase I, Phase II and Phase III trials.

4. PRODRUGS AND SOFT DRUGS (7 + 1) h

Prodrugs as drug delivery systems: Utility of prodrugs, types of prodrugs; carrier-linked prodrugs: carrier linkages for various functional groups. ***Soft drugs: concept & properties***.

REFERENCES

1. G. L. Patrick. An Introduction to Medicinal Chemistry. 5th edition, 2013. Oxford Publishers.
2. Burger’s Medicinal Chemistry and Drug Discovery and Development, Ed. D. J. Abraham and D. P. Rotella. 7th edition, 2010. Wiley-Blackwell Publishers.
3. D. Lednicer. The Organic Chemistry of Drug Synthesis. Vol. 6, 1998. Wiley-Blackwell Publishers.
4. R. B. Silverman and M. W. Holladay. The Organic Chemistry of Drug Design and Drug Action. 3rd edition, 2014. Academic Press.
5. C. O. Wilson, J. M. Beale and J. H. Block. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry. 12th edition, 2011. Published by Lipincott William & Willkins.

Semester	IV
Paper code	CHDE 0221 / 0321 /0421 / 0521
Paper title	Department elective
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

Semester	IV
Paper Code	CH0PR
Paper Title	PROJECT WORK
Number of teaching hours per week	42
Total number of teaching hours per semester	300
Number of credits	14