ST. JOSEPH'S COLLEGE (AUTONOMOUS)

BENGALURU-27

DEPARTMENT OF CHEMISTRY

SYLLABUS FOR POSTGRADUATE COURSE IN ORGANIC CHEMISTRY

2019-21

Re-accredited with 'A++' GRADE and 3.79/4 CGPA by NAAC
Recognised as "College of Excellence" by UGC

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 environment and to develop appreciation for green Chemistry.
- To prepare our students for life in the larger community.

Benchmark Statements for the Course:

- To instil 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 postgraduate (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.

SUMMARY OF CREDITS

Total no. of hrs in the semester	Credit	Number of hrs per week	Title	Code number
Semester -I				
60	4	4	Inorganic Chemistry-I	CH 7118
60	4	4	Organic Chemistry-I	CH 7218
45	3	3	Physical Chemistry-I (Quantum Chemistry)	CH 7318
60	4	4	Spectroscopy I	CH 7418
60	4	4	Principles of Chemical Analysis	CH 7518
50	1.5	4.5	Practical: Inorganic Chemistry - I	CH $7P_1$
50	1.5	4.5	Practical: Inorganic Chemistry - II	CH $7P_2$
50	1.5	4.5	Practical: Organic Chemistry - I	CH $7P_3$
50	1.5	4.5	Practical: Organic Chemistry - II	CH $7P_4$

Total hrs in the semester	Credit	Number of hrs per week	Title	Code number
Semester -II				
60	4	4	Inorganic Chemistry-II	CH 8118
60	4	4	Organic Chemistry-II	CH 8218

60	4	4	Physical Chemistry-II	CH 8318
60	4	4	Spectroscopy II	CH 8418
45	3	3	Separation Techniques	CH 8518
50	1.5	4.5	Practical: Physical Chemistry - I	CH $8P_1$
50	1.5	4.5	Practical: Physical Chemistry-II	CH $8P_2$
50	1.5	4.5	Practical: Preparation and characterization - I	CH $8P_3$
50	1.5	4.5	Practical: preparation and characterization - II	CH $8P_4$

Course Details: The details of the proposed courses for the III and IV semesters are as follows:

Total no. of hrs in the semester	**Credit**	**Number of hrs per week**	**Title**	**Code number**
Semester –III				
60	4	4	Organic Synthesis-I	OCH 9119
45	3	3	Organic Synthesis-II	OCH 9219
60	4	4	Natural products, heterocyclic chemistry and heterogeneous catalysis	OCH 9319
60	4	4	Stereochemistry and asymmetric synthesis	OCH 9419

30	2	2	Open Elective: Life's laboratories	CH OE 9618
50	1.5	4	Practical: Qualitative analysis of a binary mixture of organic compounds	OCH $9P_1$
50	1.5	4	Practical : Organic Synthesis-I (one-stage and two stage preparations)	OCH $9P_2$
50	1.5	4	Practical : Organic Synthesis-II	OCH $9P_3$
50	1.5	4	Practical : Organic Synthesis-III	OCH $9P_4$

Total no. of hrs in the semester	**Credit**	**Number of hrs per week**	**Title**	**Code number**
Semester –IV				
60	4	4	Bio-,Macro-, and Supra-molecular chemistry	OCH 0119
60	4	4	Medicinal Chemistry	OCH 0219
300	14	42	Project Work	OCH $10P_1$

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 Hrs 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	CH 7118
Paper title	INORGANIC CHEMISTRY - I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

1. CHEMICAL BONDING **13 h**

Lewis Structures: The octet rule, resonance, VSEPR model - Valence Bond Theory: homonuclear diatomic molecules (Eg: H_2 & N_2), polyatomic molecules (H_2O), hypervalence (PCl_5 & SF_6), hybridisation - Molecular Orbital Theory: Introduction (wave functions for molecular orbitals -LCAO approach - symmetry and overlap-symmetry of molecular orbitals), homonuclear diatomic molecule, heteronuclear diatomic molecule (HF, CO , BeH_2 & ICl), bond properties, bond correlations, polyatomic molecule –polyatomic molecular orbitals (Eg: NH_3), hypervalence in the context of molecular orbitals (Eg: SF_6), molecular shapes in terms of molecular orbitals- Walsh diagram (Eg: XH_2), structure and bond properties-bondlength, bondstrength, electronegativity and bond enthalpy-Pauling scale, Ketelaar triangle-Bents rule - Quadruple and agostic bonds.

2. THE STRUCTURES OF SIMPLE SOLIDS **17 h**

Unit cells and the description of crystal structures - the close packing of spheres -holes in close-packed structures - the 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, caesium-chloride, sphalerite, fluorite, wurtzite, nickel-arsenide, and rutile structures, Ternary phases $A_aB_bX_n$: perovskite and spinal structures-the rationalization of structures. Ionic radii, the radius ratio, structure maps - the energetics of ionic bonding, lattice enthalpy and the Born–Haber cycle, the calculation of lattice enthalpies, Born-Lande equation-derivation-comparison of experimental and theoretical values -the Kapustinskii equation, consequences of lattice enthalpies- Fajan's rule.

Self-study: The electronic structures of solids, the conductivities of inorganic solids, bands formed from overlapping atomic orbitals, semiconduction. Defects and nonstoichiometry - Intrinsic point defects - Schottky defect, Frenkel defect -Predicting defect types- Extrinsic point defects-F-centre Nonstoichiometric compounds and solid solutions.

3. CHEMISTRY OF THE MAIN GROUP ELEMENTS **(16 + 4) h**

Polymorphism of carbon, phosphorus and sulphur: Structure-property correlation in diamond and graphite, Intercalation compounds of graphite, carbon nanotubes-types and preparation, fullerenes-structure. Differences between 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 from 1,2-dicarba-closo-dodecaborane, sandwich structure. Borazines: Preparation, properties and structure. Difference in chemical properties between borazine and benzene, borazine derivatives (N& B substituted). Preparation of boron nitride. Phosphazenes: Classification, Cyclophosphazenes-$(NPCl_2)_3$and $(NPCl_2)_4$- preparation and structure, Linear polyphosphazenes- preparation and applications. Sulphur-nitrogen compounds: (SN)x as one dimensional conductors. Condensed phosphates – linear polyphosphates, long chain polyphosphates and metaphosphates. Polyhalides – XYn^- and Ix^- types.

***Self-study*:** Silicates- Classification and structures of ortho, pyro, chain, cyclic, sheet and three dimensional silicates.

4. ACIDS AND BASES **6 h**

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

Lux-Flood definition, systematics of Lewis acid- base interactions: Drago - Wayland equation. Factors affecting strength of Lewis and Bronsted acid- base strength 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 verses hardness and softness, symbiosis, theoretical basis of hardness and softness.

5. NONAQUEOUS SOLVENTS **4h**

Chemistry in non-aqueous media – Classification of solvents, 8leveling effect, Acid-base reactions in HF, BrF_3, N_2O_4 and molten salts, super acids- Hammet acidity function. Reactions in super critical fluids. Ionic liquids.

REFERENCES

1. Inorganic Chemistry, 5th edition, D.F. Shriver, P.W. Atkins and C.H. Langford, ELBS (Oxford Univ. Press) (2010).
2. Fundamental concepts of Inorganic chemistry, Asim K Das, volume 1, 2nd edition.
3. 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).
4. 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).

4. Basic Inorganic Chemistry - F.A. Cotton, G. Wilkinson and P. L. Gaus, John-Wiley and Sons, III edition, (1995).
5. Concise Inorganic Chemistry 5th edition, J. D. Lee, Blackwell Science, (1996).
6. Chemistry of Elements, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann (1997).
7. Fundamentals of Inorganic Chemistry, Jack Barrett and Mounir A. Malati, Harwood (1998).

Code number and Title of the paper : CH 7118; Inorganic Chemistry - I

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Chemical Bonding	13	22
2.	The Structures of Simple Solids	17	29
3.	Chemistry Of The Main Group Elements	16 + 4	34
4.	Acids and Bases	6	10
5.	Nonaqueous Solvents	4	8
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	I
Paper Code	CH 7218
Paper Title	ORGANIC CHEMISTRY - I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

1. STRUCTURE, REACTIVITY & REACTION MECHANISMS (11+4) h

Problems based on resonance, field effects, hyperconjugation, steric effects, steric inhibition of resonance.

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

Reaction mechanisms: Basic concepts: Thermodynamics and kinetics of reactions, Thermodynamic vs. kinetic control, Hammond postulate, microscopic reversibility, Marcus theory, Curtin – Hammett principle.

Reactive intermediates: Generation, structure and stability of carbenes and nitrenes.

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

Self-study: Resonance, field effects, hyperconjugation, steric effects,

Generation, structure and stability of carbocations, carbanions, carbon free radicals.

2. STEREOCHEMISTRY (15+2) h

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

Axial chirality – allenes, spiranes, biphenyls – R, S notation of these systems. Planar chirality – ansa compounds, cyclophanes. Helicity – helicenes, end substituted benzphenanthrenes.

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

Conformations of substituted ethanes and substituted cyclohexanes.

Fused rings and bridged rings – decalins, nomenclature of bridged systems, norbornanes, bicyclo [2,2,2] octane.

Effect of conformation on physical and chemical properties – acyclic and cyclic compounds.

self-study: Classification of racemic modifications, E-Z configuration notation.

3. ALIPHATIC NUCLEOPHILIC SUBSTITUTION 11 h

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 effects, 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. Susbtitution at vinyl carbon - tetrahedral and addition-elimination mechanisms.

4. ELIMINATION REACTIONS 6 h

The E2, E1, E1cB and E2C mechanisms and the spectrum of elimination mechanisms. Regioselectivity and stereochemistry of E2 and E1 reactions; effect of substrate structure, base, leaving group and medium. Substitution vs.elimination. Pyrolytic eliminations - Hofmann elimination, elimination in esters, xanthates and N–oxides - mechanism and orientaion.

5. **AROMATIC SUBSTITUTION (9+2) h**

Resonance and molecular orbital interpretation of aromaticity; aromaticity in benzenoid and non-benzenoid systems and ions.

Electrophilic substitution: Mechanistic interpretations of second substitution, orientation and reactivity, the ortho/para ratio, ipso attack, third substitution, orientation and reactivity of other ring systems like polycylic aromatic hydrocarbons, heterocyclic systems (pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyrimidine, purine and indole).

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

Reactivity – effect of substrate structure, leaving group and nucleophile; reactivity of heterocyclic systems containing 1 and 2 hetero atoms. The von Richter and Smiles rearrangements.

self-study: Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

REFERENCES

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, And Structure, Michael B. Smith and Jerry March, 6th Edn, John Wiley& Sons Inc., (2007).
2. Advanced Organic Chemistry, Part A, F. A. Carey and J. Sundberg, 5th Edn.,Springer, (2007).
3. Organic Chemistry, Paula Yurkanis Bruice, 8th Edn., Pearson Education Inc., (2017).

4. Organic Chemistry, Seyhan Ege, 3rdEdn., Houghton Miftlin Company, (1999).

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

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

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

8. Mechanism and Theory in Organic Chemistry (3rd Edition), Thomas H. Lowry, Kathleen S. Richardson, Harper & Row: New York, (1987).

9. Guidebook to Mechanism in Organic Chemistry (6th Edition), Peter Sykes, Pearson Education Limited, (1986).

Code number and Title of the paper : CH 7118; Inorganic Chemistry - I

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Structure, Reactivity & Reaction Mechanisms	15	26
2.	Stereochemistry	17	29
3.	Aliphatic Nucleophilic Substitution	11	19
4.	Elimination Reactions	6	10
5.	Aromatic Substitution	11	19
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	I
Paper code	CH 7318
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

1. QUANTUM MECHANICS FORMALISM **7 h**

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

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 h**

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 h**

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 h**

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 h**

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, I. N. Levine, Prentice Hall India (2001).

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

3. Quantum Chemistry, R. K. Prasad, New Age International (P) Ltd (1997).

Code number and Title of the paper: CH 7318; Physical Chemistry - I

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Quantum Mechanics Formalism	7	16
2.	Quantum Mechanical Treatment of Simple Systems	11	25
3.	Approximate Methods and Multielectron Atoms	8	18
4.	Theory of Angular Momentum	6	14
5.	Chemical Bonding	13	30
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	I
Paper code	CH 7418
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

1. GROUP THEORY IN CHEMISTRY **17 h**

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_{nv} point group). Applications of character tables in IR, Raman and electronic spectroscopy.

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 h**

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 h**

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 h**

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. Techniques and instrumentation.

5. ELECTRONIC SPECTROSCOPY **13 h**

Born – Oppenheimer approximation, 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 (self-study).

Application of group theory and HMO method in 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) (self-study).

REFERENCES

1. Chemical Applications of Group Theory, F.A. Cotton, Wiley Eastern (2009).
2. Molecular Symmetry, D.S. Schonland, Van Norstand, (1965).
3. Introduction to Molecular Spectroscopy, C.N. Banwell and M.McCash,

   TMH Publication,(2010).
4. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (Int. Students Edition) (1988).
5. Molecular Spectroscopy, J.D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
6. Spectroscopy, Vol 1- 3, B.P. Straughan and W. Walker, Chapman Hall (1976).
7. Modern Spectroscopy, J.M. Hollas, John Wiley (2010).
8. Vibrational Spectroscopy, D.N. Sathyanarayana, New Age International (P) Ltd. (1996).
9. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, (2001).

Code number and Title of the paper: CH 7418; Spectroscopic Methods of Analysis - I

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Group Theory In Chemistry	17	29
2.	Microwave Spectroscopy	8	14
3.	Infrared Spectroscopy	14	24
4.	Raman Spectroscopy	8	14
5.	Electronic Spectroscopy	13	22
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	I
Paper code	CH 7518
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

1. ERRORS IN CHEMICAL ANALYSIS, STATISTICAL DATA TREATMENT AND EVALUATION 10 h

Significant Figures: Rounding of numerical expression. Addition and subtraction; multiplication and division- numerical problems on above concepts.

Errors: Some important terms replicate, outlier, accuracy and precision. Errrors 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; Gausian distribution..

Sample standard deviation, sample variance, standard error of the mean, relative standard deviation, coefficient of variation, pooled standard deviation. 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 the F-test. Paired t-test for comparing individual differences. Error in hypothesis testing. Criteria for rejection of an observation - Q test. Problems. Calibration curves: least square method. Finding the least square line. (as discussed in Skoog and west). Expression for slope, intercept, standard deviation about regression. Standard deviation of the slope and intercept. Coefficient of determination

Method validation: Determination limits, calibration sensitivity. limit of quantization and linear dynamic range.

2. ACID – BASE TITRATIONS **5 h**

Basic principles: K_w pH scale, dissociation of acids and bases. Titration curves for mono functional acids and bases, pH calculations, theory of indicators. Titration curves for di, tri and polybasic acids, polyamines and amino acid systems. Fractions of phosphoric acid species as a function of pH.
Gran's plots application of acid-base titration for environmental, clinical, nutritional and industrial estimations.

3. REDOX TITRATIONS **8 h**

Nernst equation, standard & formal potentials. Titration curves, end point signals, indicators, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponent system. Adjustment of analyte's oxidation state. Application of oxidants such as permanganate, dichromate, Ce (IV), bromate, iodates, and reductants such as ferrous ammonium sulphate and ascorbic acid 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 h**

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 h**

Complexometric titrations with particular reference to EDTA titrations, suitability of polydentate ligands as titrants, expressions for the different forms of EDTA in solution as a function of pH, conditional stability constants, derivation of titration curve, 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, titrations involving monodentate ligands. Application of EDTA titration for environmental, clinical, nutritional and industrial estimations.

6. NON-AQUEOUS TITRATIONS **4 h**

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

7. GRAVIMETRIC ANALYSIS **(3+1) h**

Types of gravimetric analysis, different steps involved in gravimetric estimation. Formation and treatment of precipitates, co-precipitation, post precipitation, precipitation from homogeneous solution, important precipitating agents and their significance in inorganic analysis (Self-study).

8. KINETIC METHODS OF ANALYSIS (3+1) h

Equilibrium and kinetic methods. Rate laws, psuedo first order kinetics, types of kinetic methods, fixed time methods. Applications of catalytic and non-catalytic kinetic methods (Self-study).

9. RADIOCHEMICAL TECHNIQUES (4+1) h

Measurement of radioactivity. Different types of radiation detectors and their modes of operation. Principle, methodology and applications of isotope dilution analysis, Neutron activation analysis, PGNAA and principle of Radioimmunoassay (Self-study).

10. ABSORPTION AND EMISSION TECHNIQUES (6+1) h

Quantitative aspects of spectrochemical Measurements. Nephelometric and turbidimetric methods, Choice of method and instrumentation; DU Pont model for turbidity; EEL nephelometer (Self-study). Applications, turbidimetric titrations.

Molecular luminescence- explanation for fluorescence and phosphorescence using Jablonski diagram. (Self-study). Quantitative aspects of fluorescence. Interpretation- Internal conversion, vibrational relaxation and intersystem crossing. Fluorescence and structure with examples, effects of temperature, dissolved oxygen and solvent. Instrumentation.

Atomic absorption methods principle and Instrumentation (single and double beam) Light sources of AAS, atomization (flame and electrothermal), Interferences, detection limits, Atomic emission method (AES) Plasma – DCP and ICP techniques.(Self-study)

11. THERMAL METHODS OF ANALYSIS 2 h

Thermogravimetric analysis - differential thermal analysis; differential scanning colorimetry-thermometric titrations and applications.

REFERENCES

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

Code number and Title of the paper: CH 7518; Principles of Chemical Analysis

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Errors In Chemical Analysis, Statistical Data Treatment And Evaluation	10	17
2.	Acid – Base Titrations	5	9
3.	Redox Titrations	8	14
4.	Precipitation Titrations	4	7
5.	Complexometric Titrations	7	12
6.	Non-Aqueous Titrations	4	7
7.	Gravimetric Analysis	4	7
8.	Kinetic Methods Of Analysis	4	7
9.	Radiochemical Techniques	5	8
10.	Absorption And Emission Techniques	7	12
11.	Thermal Methods Of Analysis	2	3
Total marks excluding bonus questions			70
Total marks including bonus questions			103

PRACTICALS

Semester	I
Paper code	CH 7P1 and CH 7P2
Paper title	INORGANIC CHEMISTRY PRACTICAL I and II
Number of teaching hrs per week	9
Total number of teaching hrs per semester	99
Number of credits	1.5 +1.5

I. QUALITATIVE ANALYSIS: 11 sessions

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.

II. QUANTITATIVE ANALYSIS: 11 sessions

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	CH 7P3 and CH 7P4
Paper title	ORGANIC CHEMISTRY PRACTICAL I and II
Number of teaching hrs per week	9
Total number of teaching hrs per semester	99
Number of credits	1.5 +1.5

I. QUALITATIVE ANALYSIS: **11 sessions**

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

II. QUANTITATIVE ANALYSIS: **11 sessions**

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	CH 8118
Paper Title	INORGANIC CHEMISTRY – II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

1. METAL – LIGAND BONDING **(11+4) h**

Review of basic concepts of co-ordination chemistry (self-study). Stereochemistry 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; LFT (ACFT); MO theory-MO diagrams of octahedral complexes (including π-bonding). MO diagrams in tetrahedral complexes (self-study).

2. METAL – LIGAND EQUILIBRIA IN SOLUTION **(8+1) h**

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), potentiometry and ion-exchange methods (self-study).

3. STRUCTURE AND BONDING IN METAL COMPLEXES (13+2) h

Hydride, dihydrogen, isocyanide complexes; mononuclear and dinuclear metal carbonyls and metal carbonyl clusters, Wades rules as applied to metal carbonyl clusters (self-study), nitrosyl, dinitrogen and tertiary phosphine complexes, ligand cone angle in phosphine complexes; CO_2, SO_2 and dioxygen complexes (self-study).

Stereochemical non-rigidity, Stereoisomeriosm – chirality, optical activity, CD, ORD, Cotton effect and absolute configurations.

Concepts of Supramolecular Chemistry: Definition, nature of supramolecular interactions, host-guest interaction, molecular recognition, types of recognition, self-assembly.

Cation-binding Hosts: Concepts, cation receptors, crown ethers, cryptands, spherands, calixarenes, selectivity of cation complexation, template effect.

4. ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES 12 h

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.

5. MAGNETIC PROPERTIES OF METAL COMPLEXES (8+1) h

Origin and types of magnetic behaviour- diamagnetism, paramagnetism, ferro and antiferromagnetism, magnetic susceptibility and its measurement by the Guoy method and Faraday method (self-study), 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.

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, (1984).
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. Inorganic Chemistry, 4th Edition, D.F. Shriver and P.W. Atkins, ELBS Oxford Univ. Press. (2006).
5. Inorganic Chemistry, G. Wulfsberg, Viva Books Pvt. Ltd. (2002).
6. Inorganic Chemistry, G.L. Miessler and Tarr, 3rd edition, Pearson Education (2004).

7. Coordination Chemistry, 2nd edition, D. Banerjea, Asian Books Pvt. Ltd. (2007).
8. Chemistry of the Elements, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann, (1997).
9. An Introduction to Supramolecular Chemistry, Asim K Das and Mahua Das, CBS Publishers and Distributors Pvt. Ltd. (2017).

Code number and Title of the paper: CH 8118; Inorganic Chemistry - II

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Metal – Ligand Bonding	15	26
2.	Metal – Ligand Equilibria In Solution	9	16
3.	Structure And Bonding In Metal Complexes	15	26
4.	Electronic Spectra of Transition Metal Complexes	12	20
5.	Magnetic Properties Of Metal Complexes	9	15
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	II
Paper Code	CH 8218
Paper Title	ORGANIC CHEMISTRY – II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

1. ADDITION REACTIONS **10 h**

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 on carbonyl compounds, Wittig reaction.

Addition to carbon-hetero atom multiple bonds: Mechanisms of metal hydride reduction of carbonyl compounds, acids, esters and nitriles; addition of Grignard reagents and organolithium reagents to carbonyl compounds (self-study).

2. ALIPHATIC ELECTROPHILIC SUBSTITUTION **5 h**

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, decaboxylation of aliphatic acids; Haller-Bauer reaction.

Halogenation of aldehydes, ketones and acids, haloform reaction (self-study).

3. REARRANGEMENTS **15 h**

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 h**

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

Molecular orbital symmetry; frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems; classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams; FMO and transition state aromaticity approach; selection rules.

Electro cyclic reactions: conrotatory and disrotatory motions; 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- and 3,3-sigmatropic rearrangements;

Cope and Claisen rearrangements; Sommelet-Hauser rearrangement; Ene reaction.

5. FREE RADICAL REACTIONS AND PHOTOCHEMISTRY **10 h**

Homolysis of bonds, photochemical excitation of molecules, Beer-Lambert's law, dissipation of energy (Jablonsky diagram), singlet and triplet states (Self-study).
Generation of free radicals – thermolysis and photolysis of peroxides, peresters and azo compounds, hydrogen abstraction, chain process.
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: Cis-trans isomerisation, di-π-methane rearrangement; Norrish type I and type II cleavages; 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. Modern Synthetic Reactions, H.O. House, Benjamin, (1972).
4. Organic Chemistry, Paula Yurkanis Bruice, 7th Edn., Pearson Education, Inc., (2014).
5. Organic Chemistry, Seyhan Ege, 3rd Edn., Houghton Miftlin Company, (1999).

6. Frontier orbitals and Organic chemical reactions, Ian Fleming, John Wiley, (1980).

7. Radicals in Organic synthesis, B. Giese, Pergamon Press, (1986).

8. Organic Photochemistry, J.M. Coxon and B. Halton, 1st Edn., Cambridge University Press, London, (1974).

9. Molecular reactions and Photochemistry, C.H. Deputy and D.S. Chapman, 1st Edn. Prentice Hall India, New Delhi, (1972).

10. Mechanism and Theory in Organic Chemistry (3rd Edition), Thomas H. Lowry, Kathleen S. Richardson, Harper & Row: New York,. (1987).

Code number and Title of the paper: CH 8218; Organic Chemistry - II

Chapter Number	**Title**	**Number of teaching hours (As mentioned in the syllabus)**	**Maximum marks for which questions are to be framed from this chapter (including bonus questions)**
1.	Addition Reactions	10	17
2.	Aliphatic Electrophilic Substitution	5	9
3.	Rearrangements	15	26
4.	Pericyclic Reactions	20	34
5.	Free Radical Reactions And Photochemistry	10	17
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	II
Paper Code	CH 8318
Paper Title	PHYSICAL CHEMISTRY – II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

1. STATISTICAL THERMODYNAMICS (15+2) h

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 representatation, 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, derivation of equation for fraction of molecules occupying a given energy range,

Introduction to quantum statistics Fermi-Dirac statistics assumptions, derivation of equation for fraction of molecules occupying a given energy range,

Partition function and thermodynamic parameters—internal energy, heat capacity, free energy, chemical potential, pressure, entropy and equilibrium constant. Translational partition function, monoatomic gases,, Sackur-Tetrode equation,

Rotational, Vibrational and Electronic partition function and their evaluation from specral data Thermodynamic properties of molecules from partition function.

Self-study: Application of statistical thermodynamics: equipartition theorem, heat capacity behaviour of crystals.

2. CHEMICAL THERMODYNAMICS (13+2) h

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 ideal gas mixture.

Activity and activity coefficients: determination by solubility and emf methods, effect of temperature and pressure on fugacity and activity. Gibbs-Duhem-Margules equation; Application of Gibbs-Duhem-Margules equation, 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.

Self-study: Experimental methods for the determination of fugacity and activity coefficients. Validity of the behaviour of the solutions (laws) and their applications in separation, saturation, rectification and distillation methods. Le Chatelier principle; elementary description of phase transitions, and phase equilibria

3. NON-EQUILIBRIUM THERMODYNAMICS 6 h

Irreversible processes and steady state. Conservation of mass and energy in open systems. Entropy production – heat flow in chemical reactions. Entropy production and flow in open systems. Rate of entropy production – generalized forces and fluxes. Phenomenological equations. Onsagar reciprocity relation – electro kinetic and thermoelectric phenomena.

4. REACTION KINETICS (15 + 3) h

Review of 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 solution.

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.

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.

Self-study: Study of fast reactions by flow method, relaxation method, flash photolysis and NMR method. Listing of common organic reactions and predicting their kinetic and thermodynamic products.

5. KINETICS OF POLYMERIZATION 4 h

Kinetics and mechanism of free radical polymerization, kinetic chain length and chain transfer. Kinetics of cationic and anionic polymerization.Co-polymerization – free radical mechanism and 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. Principles of Physical Chemistry, B.R. Puri, L. R. Sharma and M. S. Pathania, Vishal Publishers co. (2017).
5. Molecular thermodynamics, Donald A. McQuarrie, John D. Simon University Science Books, California, (1999).
6. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, New age International (P) Ltd. Publishers. First edition. Reprint (2012).
7. Thermodynamics, Rajaram and J. Kuriacose, Shobhanlal Publishers (1999).

Code number and Title of the paper: CH 8318; Physical Chemistry - III

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Reaction Kinetics	18	31
2.	Kinetics And Mechanism Of Polymerization	4	7
3.	Chemical Thermodynamics	15	26
4.	Non-Equilibrium Thermodynamics	6	10
5.	Statistical Thermodynamics	17	29
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	II
Paper Code	CH 8418
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

1. UV AND VISIBLE SPECTROSCOPY **6 h**

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 h**

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 h**

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 h

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 (**Self-study**).

5. ADVANCED NMR TECHNIQUES 5h

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: ^{1}H-^{1}H correlations; an overview of the COSY experiment.

How to read COSY spectra. Problem solving (**Self-study**)

6. MASS SPECTROMETRY 8 h

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 h

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 h**

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).

Code number and Title of the paper: CH 8418; Spectroscopic Methods of Analysis – II

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	UV and Visible Spectroscopy	6	10
2.	Infrared Spectroscopy	8	14
3.	NMR Spectroscopy	17	29
4.	Carbon–13 NMR Spectroscopy	7	12
5.	Advanced NMR Techniques	5	9
6.	Mass Spectrometry	8	14
7.	Electron Paramagnetic Resonance Spectroscopy	6	10
8.	Mossbauer Spectroscopy	3	5
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	II
Paper code	CH 8518
Paper title	SEPARATION TECHNIQUES
Number of teaching hrs per week	3
Total number of teaching hrs per semester	45
Number of credits	3

1. SOLVENT EXTRACTION **5 h**

Partition coefficient-equation for batch extraction & multiple extraction, Extraction efficiency- pH effects, Extraction with metal chelator and crown ethers.

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

Types of chromatography –Theoretical principles; Retention time, retention volume, adjusted retention time, relative retention, capacity factor (retention factor) –Relation between retention time and partition coefficient –Scaling up, scaling rules-Efficiency of separation, resolution -Ideal chromatographic peaks (Gaussian peak shape)- Factors for Resolution-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, Optimum Flow Rate, A Term – multiple paths, longitudinal diffusion, Mass Transport, Extra column contributions to zone broadening -advantages of open tubular columns- isotherms and the resulting band shapes.

3. **GAS CHROMATOGRAPHY** **8 h**

Separation process in gas chromatography –schematic diagram-open tubular columns, 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-packed columns-Retention index-Temperature and pressure programming - Carrier gas-Guard columns and retention gaps-sample injections, split injection and splitless injection, solvent trapping and cold trapping, on column injection- Detectors : thermal conductivity detector, flame ionisation detector, electron capture detector, sample preparation for GC-solid phase microextraction, purge and trap, thermal desorption-Derivatisation in GC-Method development in GC.

GC-MS- transmission quadrupole mass spectrometer - selected ion monitoring.

***Self-study*:** Nitrogen phosphorous detector, flame photometric detector, photoionisation detector, Element specific plasma detectors.

4. LIQUID CHROMATOGRAPHY **8 h**

The chromatographic process-effect of small particles, scaling relation between columns, relation between number of theoretical plates and particle size, column pressure-The column, stationary phase, monolithic silica columns-Bonded stationary phases-solute column interactions-shape selectivity-The elution process, isocratic and gradient elution, selecting the separation mode, solvents, Maintaining symmetric band shape, dead volume –Injection and detection in HPLC, Detector characteristics, signal to noise ratio, detection limits, Linearity- Spectrophotometric detectors, refractive index detector, Evaporative Light scattering detector, Method development in reverse phase separation-Criteria for adequate separation-tailing of peaks- Optimisation with one solvent, optimization with two or three different solvents-choosing a stationary phase-Gradient separations- Dwell volume and Dwell time-developing a gradient separation. Derivatives for HPLC.-LC-MS.

5. LIQUID CHROMATOGRAPHIC METHODS **10 h**

Normal phase chromatography – Retention mechanism and application in isomeric separation

Ion Exchange chromatography- ion exchangers -ion exchange selectivity, selectivity coefficient, Donnan Equilibrium- Applications.

Ion Chromatography-Suppressed ion –anion and Cation chromatography-Ion chromatography without suppression-detectors-Ion pair chromatography

Molecular exclusion chromatography-the elution equation, stationary phase, molecular mass determination.

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.

Chiral separations-Chiral phases (Amylose, crown ethers and cyclodextrins)-Ligand Exchange chromatography- prikle brush type phases.

4. **SUPERCRITICAL FLUID CHROMATOGRAPHY** **1 h**

Principle -mobile phase, detectors and columns.

5. **HYDROPHILIC INTERACTION CHROMATOGRAPHY (HILIC)** **1 h**

Introduction-stationary phase for HILIC mode-mobile phase selection-mobile phase additives.

6. **THIN LAYER CHROMATOGRAPHY** **2 h**

Self-study: Preparation of thin layer plates-sample application-developing chromatogram-visualising chromatograms retention factor - high performance thin layer chromatography-forced flow planar chromatography.

7. **SAMPLE PREPARATION** **4 h**

Statistics of sampling-choosing a sample size-choosing the number of replicates.

Self-study : Dissolving samples for analysis-dissolving inorganic material by acids, dissolving inorganic material by fusion, dissolving organic substances, decomposition of organic substances-sample preparation techniques- solvent extraction, supercritical fluid extraction, preconcentration and derivatisation.

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.Super Critical Fluid Chromatography, Roger M. Smith, Royal Society of Chemistry, (1990).

Code number and Title of the paper: CH 8518; Separation Techniques

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Solvent Extraction	5	11
2.	Theoretical Aspects Of Chromatography	6	14
3.	Gas Chromatography	8	18
4.	Liquid Chromatography	8	18
5.	Liquid Chromatographic Methods	10	24
6.	Supercritical Fluid Chromatography	1	2
7.	Hydrophilic Interaction Chromatography (HILIC)	1	2
8.	Thin Layer Chromatography	2	5

9.	Sample Preparation	4	9
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	II
Paper Code	CH 8P1 and CH 8P2
Paper Title	PHYSICAL CHEMISTRY PRACTICAL I AND II
Number of teaching hrs per week	9
Total number of teaching hrs per semester	99
Number of credits	1.5 + 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. Degree of hydrolysis of aniline hydrochloride.
7. Saponification of ethyl acetate by conductometric method.
8. Evaluation of rate constant of first order reaction by potentiometry.
9. Estimation of urea by enzyme hydrolysis using conductance method
10. Experiment to be designed by students.

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. Determination of dissociation constant of a weak acid or weak base by conductometry.
3. Determination of Onsagar parameters for a strong electrolyte by conductometry.
4. Titration of silver nitrate against potassium chloride/bromide/ iodide, calculation of the solubility product of silver chloride/bromide/iodide.
5. Titration of a weak acid against a strong base using quinhydrone electrode and calculation of pKa values of the weak acid.
6. Titration of a mixture of strong and weak acids potentiometrically and the determination of the composition of the mixture.
7. Determination of activity coefficient of an electrolyte by potentiometry.
8. Determination of the Fe/ Cu in different matrices by colorimetry.
9. Determination of pK_a of indicators by colorimetry.
10. 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	CH 8P3 and CH 8P4
Paper Title	Synthesis and Characterization of Compounds I and II
Number of teaching hrs per week	9
Total number of teaching hrs per semester	99
Number of credits	1.5 +1.5

I Inorganic Compounds:

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

II Organic Compounds:

6. Preparation of anthrone from anthracene.
7. Preparation of anthranilic acid from phthalic acid.
8. Preparation of benzanilide from benzophenone.
9. Preparation of benzilic acid from benzoin.
10. Preparation of NBS from succcinic acid and its application in allylic bromination.
11. Synthesis of stilbene.
12. Resolution of a racemic mixture by fractional crystallization

13. 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 costing (from the point of view of Green chemistry)

    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	OCH 9119
Paper title	ORGANIC SYNTHESIS-1
Number of teaching hrs per week	04
Total number of teaching hrs per semester	60
Number of credits	04

1. PRINCIPLES OF GREEN CHEMISTRY **6h**

General introduction to green chemistry, need for green chemistry, limitations/obstacles.

Important aspects of green chemistry: less hazardous chemical synthesis, use of green catalysts and solvents and solvent-free synthesis, atom economical synthesis, metal-free synthesis using organocatalysts, reducing hazardous reaction conditions (microwave, ultrasonic, mechanochemical synthesis), avoiding multi-step synthesis or energy minimization (one-pot multicomponent synthesis, reducing number of by-products, recyclability of catalyst).

Green solvents: use of water and supercritical fluids as solvent, solvent-free synthesis (one example for each condition). Use of green catalysts in organic synthesis and its reusability.

Energy minimization: Microwave (synthesis of benzyl alcohol from benzyl chloride), ultrasonic synthesis, mechanochemistry with one example each. (options as Hoffmann elimination, methyl benzoate to benzoic acid, Diels-alder reaction).

Designing green synthesis for the following reactions with the help of one example each; rearrangement reactions (e.g. benzil-benzilic acid rearrangement), electrophilic substitution reactions (e.g. bromination of acetanilide). Comparison of greenness of reaction with conventional methods.

2. IMPORTANT REACTIONS IN ORGANIC SYNTHESIS **(7+1) h**

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

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

C-N bond formation: Barton reaction

Self-study: Perkin reaction, Dieckmann condensation, Claisen ester condensation, Knoevenagel condensation.

3. OXIDATION-REDUCTION (12+1) 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, Pummerer reaction, Willgredot reaction, Corey-Bakshi-Shibata reaction and Tischenko reaction.

4. MULTI-COMPONENT REACTIONS (3+1) h

Synthesis and applications of multi-component reactions. Advantages and examples including Ugi, Passerini, Biginelli and Mannich reaction. Domino reaction: synthesis of isoquinolines using Knoevenagel/Michael approach.

Self-study: Applications of Ozone and Osmium tetroxide as oxidants, Birch and Clemmenson reduction.

5. ORGANOMETALLICS IN ORGANIC SYNTHESIS (7+2) h

Organolithium compounds - application in deprotonation of C-H bonds, enantioselective lithiation, ortho directing effect, addition to multiple bonds (anionic polymerization), substitution, transmetallation. Organomagnesium compounds (Grignard reagent), applications in the synthesis of organic and organometallic compounds, application of organozinc compounds (ZnR_2) in Simmons-Smith reaction, Gilman reagent mediated organic synthesis using Me_2CuLi as an example.

6. TRANSITION METAL COMPLEXES (HOMOGENEOUS CATALYSIS) IN ORGANIC SYNTHESIS (11+1) h

Catalytic cycle and key reaction steps in homogeneous catalysis-ligand dissociation, association, oxidative addition-reductive elimination, insertion/de-insertion.

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, 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). *Self-study:* 18- and 16-electron rules. Current trends in homogeneous catalysts.

7. C-H BOND ACTIVATION IN ORGANIC SYNTHESIS 8h

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

Mechanism of different types of C-H activation with suitable examples: radical-mediated, nickel-catalyzed, cobalt-catalyzed, iron-catalyzed, rhodium-catalyzed, copper-mediated, palladium-catalyzed C-H bond activation reactions.

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

REFERENCES

1. Ahluwalia V. K. and Kidwai M. R. Trends in Green Chemistry, 2005, Anamalaya Publishers.
2. Anastas P. T. and Warner J. K. Oxford Green Chemistry. Theory and Practical. 1998, University Press.
3. M. B. Smith and J. March. March's Advanced Organic Chemistry, 6th edition, 2007, John Wiley & Sons Inc.
4. F. A. Carey and R. J. Sundberg. Advanced Organic Chemistry. Part B: Reactions and synthesis. 5th edition, 2007, Springer publishers.
5. W. Carruthers and L. Coldham. Modern Methods of Organic Synthesis, 4th edition, Cambridge University Press.
6. P. Sykes. Mechanism in Organic Chemistry, 6th edition, 2003, Pearson Publishers.
7. J. Clayden, N. Greeves, S. Warren and P. Wothers. Organic Chemistry. Oxford Press.
8. Organotransition Metal chemistry by J. F. Hartwig, University Science Books, 2010.
9. Organic Chemistry by J. Clayden, N. Greeves and S. Warren, Oxford University Press, 2012

10. Basic Organometallic Chemistry 2nd Edition by A. J Elias, B. D. Gupta, Universities Press 2013.
11. Organometallics and Catalysis by Manfred Bochmann, Oxford University Press, 2015
12. Organometallics 3rd Edition by Christoph Elschenbroich Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2006
13. The Organometallic Chemistry of Transition Metals, R. H. Crabtree 6th edn. John Wiley & Sons 2014.
14. C-H bond activation in organic synthesis. Ed. J. J. Li. 2017. CRC Press Publishers.
15. C-H activation. Ed. J. -Q. Yu and Z. Shi. 2010. Springer Publishers.

Code number and Title of the paper: OCH 9119; Organic synthesis-I

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Principles of green chemistry	6	10
2.	Important reactions in organic synthesis	8	14
3.	Oxidation-reduction	13	22
4.	Multi-component reactions	4	7
5.	Organometallics in organic synthesis	9	15
6.	Transition metal complexes (homogeneous catalysis) in organic synthesis	12	21
7.	C-H bond activation in organic synthesis	8	14
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	III
Paper code	OCH 9219
Paper title	ORGANIC SYNTHESIS-II
Number of teaching hrs per week	03
Total number of teaching hrs per semester	45
Number of credits	03

1. RETROSYNTHESIS (28+2) h

The Disconnection approach: Basic principles; introduction to synthons and synthetic equivalents; chemo selectivity.

Protecting groups: protection of alcohols, carbonyl compounds, amines and carboxylic acids.

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

Synthesis of aromatic compounds; reversal of polarity, cyclization reactions; amine synthesis.

One group C-C and two group C-C disconnections: carbonyl compounds, alkene synthesis, use of acetylides and aliphatic nitro compounds in synthesis, Diels-Alder reactions; 1,3-, and 1,5-, difunctionalized compounds, α,β-unsaturated carbonyl compounds, carbonyl ,condensations, Michael addition and Robinson annulation.

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

Convergent synthesis: Differences between convergent and linear synthesis. Advantages of convergent synthesis over linear synthesis.

Convergent synthetic strategy for Ferruginol, α-Bisabolene and Lycorane

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 15h

REFERENCES:

1. Organic Synthesis: The Disconnection Approach by Stuart Warren (Wiley India)
2. Work Book 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, 5th Edn.

Code number and Title of the paper: OCH 9219; Organic synthesis-II

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Retrosynthetic analysis	30	69
2.	Review article based modern aspects of organic chemistry	15	34
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	III
Paper code	OCH 9319
Paper title	NATURAL PRODUCTS, HETROCYCLIC CHEMISTRY AND HETEROGENEOUS CATALYSIS
Number of teaching hrs per week	04
Total number of teaching hrs per semester	60
Number of credits	04

TERPENES **(9+1) h**

Structural elucidation, biosynthesis and synthesis of α-pinene (an example of bicyclic monoterpene), farnesol (an example of acyclic sesquiterpene) and abeitic 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.

Self-study: Classification, nomenclature, occurence, isolation of terpenes. Isoprene rule, stereochemistry of citral, limonene, menthol and borneols.

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)

Self-study: Definition, nomenclature, occurence and classification of alkaloids.

PORPHYRINS AND VITAMIN B_{12} **4h**

Structural elucidation, biosynthesis and synthesis of Haemin and Vitamin B_{12} (Synthesis of Vitamin B_{12} from Cobyric acid)

INSECT PHEROMONES **(2+1) h**

Introduction and classification. Stereoselective synthesis of bombykol and 3,11-dimethyl-1,2-nonacosanone.

Self-study: Pheromones in pest control.

PROSTAGLANDINS **6h**

Introduction, nomenclature, classification and biological role of prostaglandins.

Biosynthesis of prostaglandins, conversion of arachidonic acid to prosatgalndins, prostacyclins and thromboxanes.Structural elucidation and stereochemistry of PGE_1.

Synthesis of PGE_1 by Corey's approach. Synthesis of PGE_2 by Upjohn's approach.

Synthesis of prostacyclin I_2 and Thromboxane B_2.

HETREOCYCLIC CHEMISTRY **(19+1) h**

Three and four membered oxygen and nitrogen containing heterocycles- name and structure (self study)

Five- and six-membered heterocycles with one heteroatom: synthesis and reactions of pyrrole, furan, thiophene, quinoline, isoquinoline, indole.

Five- and six-membered heterocycles with two or more hetero atoms: synthesis and reactions of 1,2,3-triazole, 1,2,4-triazole, 1,2,4-oxadiazole, 1,3,4-oxadiazole, diazines, triazines, tetrazines and thiazines.

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

APPLICATION OF HETROGENEOUS CATALYSIS IN ORGANIC SYNTHESIS **10h**

Characteristics of heterogeneous catalysts, active sites in catalysts (single and multiple centres, particle size *vs* number of active sites), role of supports; catalyst-support interaction, Langmuir-Hinshelwood mechanism and Langmuir-Riedell mechanism (*no derivation*)

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

Supported catalysts (acid, base and metal): Impregnation/encapsulation of active species on high surface area supports, (Keggin on Zirconia, Pt/C, Cr_2O_3/*gamma*-Al_2O_3, isomerization of *n*-alkanes to branched alkanes, alkane dehydrogenation and dehydrocyclization)

Zeolites: acid and base catalysis, pore size and channel variation with Si/Al ratio (reactant and product selectivity-para xylene synthesis), ion exchange (CsX, CsA, CsY- condensation and styrene synthesis)

Oxidation catalysts: mixed oxides (MoO_3 or V_2O_5/Al_2O_3- synthesis of nicotinic acid, phthalic anhydride, TS-1, epoxidation), transition metal catalysts (with examples)

Heterogenising aspects of homogeneous transition metal complexes: Immobilization of transition metal complex catalysts on inorganic supports (i.e., anchored catalysts, examples), active sites and leaching mechanism.

REFERENCES:

1. Chemistry of natural products, Kalsi.
2. Chemical Aspects of Biosynthesis, J. Mann
3. 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)
4. Terpenes , J. Verghese (Tata Mc graw-Hill, New Delhi, 1982)
5. Chemistry of terpenes and terpenoids, A. Newman (Academic press, London,1975)
6. Organic Chemistry by I. L. Finar, vol II(6thEdn,Longman, 1992)
7. Chemistry of natural products vol I and II by O.P. Aggarwal (Goel Publishing house, 6th edn,1982)
8. Organic Chemistry of Natural products Vol I and II by Gurudeep R. Chatwal, ed: M. Arora (Himalaya publishing House, New Delhi, 2015)
9. Chemistry of Natural Products: A Unified Approach by N.R. Krishnaswamy (University press, London, 1999)
10. The Colours of Life: An Introduction to the Chemistry of Porphyrins and Related Compounds by L.R. Milgrom (Wliey Chichester, 1995)
11. Total Synthesis of Steroids by Akhaun and Titov (Jerusalem,1969)
12. Total Synthesis of Natural products: The Chiral Approach, Vol III by S. Hanessian (Pergamon Press, 1983)
13. Medicinal Natural products: A Biosynthetic Approach by P.M. Dewick (John Wiley, Chichester,1997)
14. S. P. Bhutani. Organic Chemistry: Selected topics. 2008, Ane Books.
15. J. A. Joule, K. Mills, G. F. Smith. Heterocyclic Chemistry. 5th edition, 2010. John Wiley and Sons Ltd.
16. R. M. Acheson. An introduction to Heterocyclic Chemistry. 3rd edition, 2008. Wiley India Pvt. Ltd.
17. Modern Heterogeneous Catalysis, an Introduction by R. A. van Santen, Wiley VCH, 2017-1)

18. Gerard, V. S.; Ferenc, N. Heterogeneous Catalysis in Organic Chemistry; Academic Press; New York. 1st ed, 2006.
19. Heterogeneous Catalysis for the Synthetic Chemist, R. L. Augustine, Dekker, New York, 1995.
20. Heterogeneous Catalysis and Fine Chemicals IV, H. U. Blaser, A. Baiker, and R. Prins (Eds.), Elsevier, Amsterdam, 1997.
21. Somorjai, G. A., Introduction to Surface Chemistry and Catalysis, Wiley, New York, 1994.
22. J. H. Sinfeltin G. Ertl, H. Kneozinger, J.Weitkamp (eds.): Handbook of Heterogeneous Catalysis, Vol. 4, Wiley-VCH, Weinheim 1997
23. A.Corma, H. Garcia, Chem. Rev. 2003, 103, 4307.
24. A. Corma Chem. Rev. 2018, 118, 10, 4981-507.

Code number and Title of the paper: OCH 9319; Natural products, hetrocyclic chemistry and heterogeneous catalysis

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Terpenes	10	17
2.	Alkaloids	7	13
3.	Porphyrins and vitamin B_{12}	4	7
4.	Insect pheromones	3	5
5.	Prostaglandins	6	10
6.	Heterocyclic chemistry	20	34
7.	Application of heterogeneous catalysis in organic synthesis	10	17
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	III
Paper code	OCH 9419
Paper title	STEREOCHEMISTRY AND ASYMMETRIC SYNTHESIS
Number of teaching hrs per week	04
Total number of teaching hrs per semester	60
Number of credits	04

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

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

Stereochemistry of fused, bridged and caged systems: Paddlanes and propellanes; cantenanes, rotaxanes, knots, and Möbius strips; cubane, tetrahedrane, dodecahedrane, adamantane and Buckminsterfullerene

Conformation of unsaturated acyclic and miscellaneous compounds.

EFFECT OF CONFORMATION ON REACTIVITY **8h**

Diastereomer equilibria in acyclic systems.

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

ASYMMETRIC SYNTHESIS **17h**

'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. Addition of allylmetal and allylboranes to carbonyl group. Diastereoselection in cyclic systems: Nucleophilic addition to cyclic ketones (formation of axial and equatorial alcohols, catalytic hydrogenation, alkylation, diastereoselective oxidations and stereoselective cyclization of poylenes).

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

Enantioselective alkylation of ketones via hydrazones. Enantioselective alkylation with chiral PTC. Enantioselective Michael addition. Enantioselective intramolecular aldol condensation. Use of (+)- and (–)- DET in asymmetric epoxidation.

Polymer-bound chiral catalysts in asymmetric induction. Asymmetric amplification.

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.

(*Self-study: chiral chromatography for enantiomeric resolution*)

CHIROPTICAL PROPERTIES 12h

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; exciton chirality; 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. Circular Dichroism: Principles and Applications, N. Berova, K. Nakanishi, R. W. Woody, 2nd Edn., John Wiley & Sons Inc., 2000.

Code number and Title of the paper: OCH 9419; Stereochemistry and asymmetric synthesis

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Stereochemistry of unsaturated acyclic, fused, bridged and caged systems	14	24
2.	Effect of conformation on reactivity	8	14
3.	Asymmetric synthesis	17	29
4.	Chiral resolution techniques	8	14
5.	Chiroptical properties	12	22
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	III
Paper code	CH OE 9618
Paper title	Open Elective: Life's laboratories
Number of teaching hrs per week	2
Total number of teaching hrs 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).

3. Biochemistry - Gareth and Grisham, Saunders College Publishing.

4. New trends in green chemistry - Ahluwalia and Kidwai, Anamaya Publishers, New Delhi.

5. Forensic Chemistry - Suzanne Bell - Pearson Publishers.

Code number and Title of the paper: CHOE 9618; Life's laboratories

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Chemistry and society	2	3
2.	Molecular gastronomy	5	9
3.	Forensic chemistry	5	9
4.	Molecular processes	3	4
5.	Green chemistry and the industry	5	9
6.	Research based pedagogy tools	10	18
Total marks excluding bonus questions			35
Total marks including bonus questions			52

THIRD SEMESTER

PRACTICAL PAPERS

Semester	III
Paper Code	$OCH9P_1$
Paper Title	PRACTICAL : QUALITATIVE ANALYSIS OF A BINARY MIXTURE OF ORGANIC COMPOUNDS
Number of teaching hrs per week	4
Total number of teaching hrs per semester	50
Number of credits	1.5

The components of the given binary mixture would be separated by suitable solvent extraction and each of the components will be analysed systematically to identify them. (11 sessions)

Semester	III
Paper Code	$OCH9P_2$
Paper Title	PRACTICAL : ORGANIC SYNTHESIS-I (ONE-STAGE AND TWO STAGE PREPARATIONS)
Number of teaching hrs per week	4
Total number of teaching hrs per semester	50
Number of credits	1.5

This practical course involves single-step and multistep organic synthesis, characterization of the products through relatively simple techniques like thin layer chromatography, melting point measurement. It also includes spectral analysis of the compounds.

1. Oxidation of cyclohexanal to adipic acid (2 sessions)
2. Preparation of S-benzylisothiouroniumchloride (2 sessions)
3. Preparation of 2,4,6 tribromoaniline (2 sessions)
4. Synthesis of 2,4-dinitrophenylhydrazine from chlorobenzene (2 sessions)
5. Synthesis of hydantoin (3 sessions)
6. Any other practicals

Semester	III
Paper Code	$OCH9P_3$
Paper Title	PRACTICAL : ORGANIC SYNTHESIS-II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	50
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, purification and characterization of a synthetic resin. (3 sessions)
2. Synthesis and characterization of a low molecular weight organic gelator. (2 sessions)
3. Shape-selective properties of Zeolite Na-Y catalyst. (2 sessions)
4. Crown ether as a phase transfer catalyst (2 sessions)
5. Synthesis of tetrahydrocarbazole from cyclohexanone-Fischer indolization (2 sessions)
6. Any other practicals

Semester	III
Paper Code	$OCH9P_4$
Paper Title	PRACTICAL : ORGANIC SYNTHESIS-III
Number of teaching hrs per week	4
Total number of teaching hrs per semester	50
Number of credits	1.5

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 **11 sessions**

1. Training on purification and instrumentation. (1 session)
2. Synthesis of benzimidazole in aqueous medium. (3 sessions)
3. Suzuki coupling reaction using $Ni(PPh_3)_2Cl_2$ catalyst. (3 sessions)
4. Microwave assisted nitration of phenol using copper nitrate (2 sessions)
5. Solvent-free reductive amination using mortar and pestle (2 sessions)
6. Any other practicals

REFERENCES

1. Analytical Chemistry-An introduction; Skoog, West, Holler and Crouch; seventh edition Saunders College Publishing, (1999).
2. Textbook of Practical Organic Chemistry, A I Vogel, ELBS (1973).
3. Chromatography, C.G. Sharma Krishna Prakashana Media (1997).

FOURTH SEMESTER

THEORY PAPERS

Semester	IV
Paper code	OCH 0119
Paper title	BIO-, MACRO-, SUPRA-MOLECULAR CHEMISTRY
Number of teaching hrs per week	04
Total number of teaching hrs per semester	60
Number of credits	04

1. BIOMOLECULES **(11+4) h**

Carbohydrates: Types of naturally occurring sugars (self-study). Deoxy sugars, amino sugars, branched chain sugars. Methyl ethers and acid derivatives of sugars (self-study). General methods of structure and ring size determination with particular reference to maltose. Oxidation and reduction reactions of monosaccharides. Synthesis and Degradation of Monosaccharides (Kiliani-Fischer Synthesis, The Ruff degradation). Structure, degradation and biological functions of starch, cellulose and chitin. Peptides: General idea of the peptide linkage and primary structure of proteins and its determination; Sanger and Edman methods (self-study); Cleavage of peptide bond by chemical and enzymatic methods. Peptide synthesis- Protection of amino group and carboxyl group as alkyl and aryl esters. Use of DCC, EEDQ, HOBt and active esters, acid halides, anhydrides in peptide bond formation reactions. Deprotection and racemization in peptide synthesis. Solution and solid phase techniques.

Nucleic acids: Purine and pyrimidine bases. Structure of nucleosides and nucleotides (self-study). Synthesis of nucleosides and nucleotides. Methods of formation of internucleotide bonds (DCC, phosphotriester approach).

2. POLYMER CHEMISTRY **(11+4) h**

Self study: Introduction: Definition of polymer, monomer, repeat unit, polymerization; nomenclature-IUPAC, non-IUPAC, structure-based, and trade names; classification of polymers based on source; polymer composition; molecular structure (linear, branched, cross-linked, block); stereochemistry of repeating units (tacticity in polymers).

Synthesis of polymers: Chemistry of radical, anionic and cationic polymerization; Ziegler–Natta catalysts; copolymerization, polycondensation polymerization. reactivity ratios, thermodynamic aspects of polymerization, mechanism of living radical polymerizations: nitroxide mediated polymerization (NMP), metal-catalyzed living radical polymerization, reversible addition-fragmentation chain transfer (RAFT) radical polymerization, coordination polymerization, ring opening polymerization, click chemistry. Methods of polymerization: Bulk, solution, suspension and emulsion polymerizations.

Characterization of polymers: molecular weight studies (mass spectroscopy and DLS/SLS) and molecular weight distribution, polydispersive index. Polymer behavior, crystallinity, rheology, thermal behavior, Glass transition temperature, factors influencing the glass transition; plasticizers. Biodegradable polymers.

3. SUPRAMOLECULAR CHEMISTRY (29+1) h

Introduction: Definition and development of supramolecular chemistry- lock and key analogy**,** cooperativity-pre-organisation- complementarity-thermodynamic, kinetic selectivity-nature of supramolecular interactions- solvation effects, supramolecular concepts and design.
Host-guest Chemistry: Synthesis: The template effect and high dilution.

Cation-binding: crown ethers, cryptands, spherands, calixarenes (review-recall), proton binding, Lariat ethers, podands, alkalides, electrides and siderophores.
Anion binding: Concepts in anion host design, different types of anion hosts.
Simultaneous cation and anion binding
Molecular Recognition: hydrogen bonds, hydrophobic interactions. Guest binding by cavitands-calixarenes, resorcarenes, glycourils, cyclodexdrins; molecular clefts, tweezers, cyclophanes, cryptophanes, carcerends and hemicarcerends

Dendrimers: Synthesis-divergent and convergent methods, host-guest chemistry of dendrimers and applications

Supramolecular Catalysis: Cyclodexdrin as enzyme mimics
Self-Assembly: Self-assembly in synthetic systems: Kinetic and thermodynamic considerations, pi-

electron donor-acceptor systems, transition metal directed assemblies, hydrogen bond assemblies, anion directed assemblies, catenanes, rotaxanes, helicates, helical assemblies and molecular knots. Solid state supramolecular chemistry: Clathrate hydrates, urea, thiourea clathrates, inclusion compounds (tri-*o*-thymotide, cyclotriveratrylene), Intercalation compounds

Crystal engineering: Tectons and synthons, role of hydrogen bond synthons, coordination polymers.

Applications of supramolecular chemistry–Sensors, switches and molecular machinery

REFERENCES

1. Organic chemistry Vol.II, I. L. Finar, Longman, 6th Edn., (1992).

2. Organic Chemistry, J. Clayden, N. Greeves and S. Warren, Oxford University Press, 2nd Edn., (2012)

3. Biochemistry, D. Voet and J. G. Voet, John Wiley and Sons, 4th Edn., (2010).

4. Principles of Polymerization, G. Odian, Wiley-Interscience, 4th Edn., (2004).

5. Text book of Polymer Science, F. W. Billmeyer, John Wiley and sons, 3rd Edn. (1984).

6. Introduction to synthetic polymer, I. M. Cambell, Oxford University Press, 2nd Edn., (2000).

7. Principles of Polymer Science, P. Bahadur and N. V. Sastry, CRC Press, (2002).

8. Plastics of the Future? The impact of Biodegradable Polymers on the Environment and on Society: T. P. Haider, C. Volker, J. Kramm, K. Landfester, F. R. Wurm; Angew. Chem. 2019, 58, 50.

9. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John Wiley, 2nd Edn., (2009).

10. Core Concepts in supramolecular Chemistry and Nanochemistry, J. W. Steed, T. R. Turner and K. J. Wallace, John Wiley & Sons, (2007).

11. Supramolecular Chemistry, L.-M. Lehn, VCH, 1995

12. Crystal Design: Structure and Function, G. R. Desiraju (Ed.), John Wiley and Sons, (2003).

Code number and Title of the paper: OCH 0119; Bio-, macro-, supra-molecular chemistry

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Biomolecules	15	26
2.	Polymer chemistry	15	26
3.	Supramolecular chemistry	30	51
Total marks excluding bonus questions			70
Total marks including bonus questions			103

Semester	IV
Paper code	OCH 0219
Paper title	MEDICINAL CHEMISTRY
Number of teaching hrs per week	04
Total number of teaching hrs per semester	60
Number of credits	04

1. MOLECULAR ASPECTS OF DRUG ACTION (11+1) h

Drug, API, drug additives (brief account of classification and meaning of different additives), 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}, ID_{50} and EC_{50}.

Self-study: Drug additives (brief account of classification and meaning of different additives).

2. CLASSIFICATION OF DRUGS BASED ON THERAPEUTIC ACTION 28 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: Introduction, 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: Introduction, 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 class 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, anti-metabolites- 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

Difference between drugs and medicines. Procedure followed in drug design: drug discovery 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.

Self-study*:* Difference between drugs and medicines. Lipinsky's rule of 5.

4. PRODRUGS AND SOFT DRUGS 8h

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.

Code number and Title of the paper: OCH 0219; Medicinal chemistry

Chapter Number	Title	Number of teaching hours (As mentioned in the syllabus)	Maximum marks for which questions are to be framed from this chapter (including bonus questions)
1.	Molecular aspects of drug action	12	21
2.	Classification of drugs based on therapeutic action	28	47
3.	Stages of drug development and drug discovery	12	21
4.	Prodrugs and soft drugs	8	14
Total marks excluding bonus questions			70
Total marks including bonus questions			103