ST. JOSEPH'S UNIVERSITY

BENGALURU - 27

SCHOOL OF CHEMICAL SCIENCES

DEPARTMENT OF CHEMISTRY

SYLLABUS FOR POSTGRADUATE COURSE
M.Sc. ANALYTICAL CHEMISTRY

2022-2024

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

FROM 2022 ONWARDS

Department of Chemistry

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

Mission statement:

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

Benchmark Statements for the Course:

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

Teaching-Learning:

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

Co-curricular Activities:

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

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

SUMMARY OF CREDITS

SEMESTER	PAPER CODE AND TITLE	NO. OF TEACHING HOURS/week	NO. OF CREDITS	TOTAL MARKS
SEMESTER I				
THEORY				
Paper I	CH7121: Inorganic Chemistry - I	4	04	100
Paper II	CH7221: Organic Chemistry - I	4	04	100
Paper III	CH7321: Physical Chemistry - I	3	03	100
Paper IV	CH7421: Spectroscopy -I	4	04	100
Paper V	CH7521: Principles of Chemical Analysis	4	04	100
PRACTICAL				
Paper I	CH7P1 Inorganic Chemistry Practical I	4	1.5	50
Paper II	CH7P2 Inorganic Chemistry Practical II	4	1.5	50
Paper III	CH7P3 Organic Chemistry Practical I	4	1.5	50
Paper IV	CH7P4 Organic Chemistry Practical II	4	1.5	50
		TOTAL	25	500
SEMESTER II				
THEORY				
Paper I	CH8121: Inorganic Chemistry II	4	04	100
Paper II	CH8221: Organic Chemistry II	4	04	100
Paper III	CH8321: Physical Chemistry II	4	04	100
Paper IV	CH8421: Spectroscopy II	4	04	100
Paper V	CH8521: Separation Techniques	3	03	100
Note: Students can choose one of the departmental elective from Paper V-A or V-B				

PRACTICAL				
Paper I	CH8P1 Physical Chemistry Practical I	4	1.5	50
Paper II	CH8P2 Physical Chemistry Practical II	4	1.5	50
Paper III	CH8P3 Preparation and characterization - I	4	1.5	50
Paper IV	CH8P4 Preparation and characterization - II	4	1.5	50
		TOTAL	25	600

SEMESTER	**PAPER CODE AND TITLE**	**NO. OF TEACHING HOURS**	**NO. OF CREDIT S**	**TOTAL MARKS**
SEMESTER III				
THEORY				
Paper I	CH9122: Biological Chemistry	4	4	60
Paper II	CH9222: Organometallic Chemistry	4	4	60
Paper III	CH9322: Electrochemistry and Electroanalytical Techniques	3	3	45
Paper IV	CH9422 Solid State Chemistry	4	4	60
Paper V (OE)	CHOE 9521: Open elective: Life's laboratories CHOE 9622: Culinary Chemistry	2	2	30
Note: Students choose open elective from other departments.				

PRACTICAL				
Paper I	CH9P1: Applied Analysis-I	4	1.5	50
Paper II	CH9P2: Applied Analysis-II	4	1.5	50
Paper III	CH9P3: Advanced Methods of Analysis –I	4	1.5	50
Paper IV	CH9P4: Advanced Methods of Analysis –II	4	1.5	50
		TOTAL	**6**	**200**
SEMESTER IV				
Paper I	CH0121: Applied Analysis	4	4	60
Paper II	Dept Electives CHDE 0221: Chemistry of Materials CHDE 0321: Green Chemistry and Diversity of its Applications CHDE 0421: Forensic Chemistry CHDE 0521: Supramolecular Chemistry	4	4	60
	CH0PR PROJECT WORK	**42/week**	**14**	**100**
	IGNITORS/ OUTREACH		**04**	
Total No. of Credits : 26				
KEY WORDS: DE – Departmental Elective and OE – Open Elective				

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

CREDITS FOR M.Sc. CHEMISTRY						
I -II SEMESTER						
	T/P	**Number Of Teaching hours Per Week**	**CREDITS**	**Total Teaching hours in a semester**	**TOTAL CREDITS IN ONE SEMESTER**	**TOTAL CREDITS IN ALL SEMESTERS**
Optional Subjects					25	25 x 2 = 50
A	T	4	4	60		
B	T	4	4	60		
C	T	4	4	60		
D	T	4	4	60		
E	T	3	3	45		
Practical-I	P	4.5	1.5	50		
Practical –II	P	4.5	1.5	50		
Practical-III	P	4.5	1.5	50		
Practical –IV	P	4.5	1.5	50		
III SEMESTER						
Optional Subjects					25	25
A	T	4	4	60		
B	T	4	4	60		
C	T	3	3	45		
D	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
Dept. elective	T	4	4	60		
PROJECT	P	42	15	100		
IGNITORS			2			
TOTAL						**100**

FIRST SEMESTER

THEORY PAPERS

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

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

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

1. **CHEMICAL BONDING** **13 hrs**

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

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

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

Defects and nonstoichiometry - Intrinsic point defects - Schottky defect, Frenkel defect - Predicting defect types- Extrinsic point defects-F-centre, nonstoichiometric compounds.

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

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

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

4. ACIDS AND BASES 6 hrs

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

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

5. NONAQUEOUS SOLVENTS 4 hrs

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

REFERENCES

1. Inorganic Chemistry, M. T. Weller, J. P. Rourke, T. L. Overton and F.A. Armstrong, 7th edition, Oxford Univ. Press, (2018).

2. Inorganic Chemistry, Catherine E. Housecroft and Alan G. Sharpe, 5th edition, Pearson Education Limited, (2018).

3. Principles of Inorganic Chemistry, B. W. Pfennig, 2nd edition, John Wiley & Sons Inc. (2022).

4. Inorganic Chemistry, G. L. Miessler, P. J. Fischer and D. A. Tarr, 5th edition, Pearson Education Limited, (2014).

5. Inorganic Chemistry, J. E. House, 3rd edition, Academic Press (2020).

6. Chemistry of the Non-Metals, R. Steudel, Walter de Gruyter GmbH (2020).

7. Fundamental concepts of Inorganic chemistry, 2nd edition Asim K Das, volume 1,.(2014)

8. Reactions in supercritical fluids- a Review, Bala Subramaniam and Mark A. McHugh Ind. Eng. chem. Process Design and development. Vol 25. Issue 1. Pages 1-12, (1986).

9. Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, J.E. Huheey, E.A. Keiter and R.L. Keiter, Okhil. K.Medhi, Pearson Education Asia Pvt. Ltd. (2006).

8. Basic Inorganic Chemistry - F.A. Cotton, G. Wilkinson and P. L. Gaus, John-Wiley and Sons, III edition, (1995).

9. Concise Inorganic Chemistry, 5th edition, J.D.Lee, Blackwell Science, (1996).

10. Chemistry of Elements, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann (1997).

Semester	I
Paper Code	CH7221
Paper Title	ORGANIC CHEMISTRY - I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

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

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

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

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

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

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

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

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

2. STEREOCHEMISTRY 15+2 = 17 hrs

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

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

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

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

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

3. ALIPHATIC NUCLEOPHILIC SUBSTITUTION **11 hrs**

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

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

4. ELIMINATION REACTIONS **6 hrs**

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

5. AROMATIC SUBSTITUTION **9+2=11 hrs**

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

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

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

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

REFERENCES

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

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

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

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

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

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

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

Semester	I
Paper code	CH7321
Paper title	PHYSICAL CHEMISTRY – I (Quantum Chemistry)
Number of teaching hrs per week	3
Total number of teaching hrs per semester	45
Number of credits	3

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

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

1. QUANTUM MECHANICS FORMALISM 7 hrs

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

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

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

2. QUANTUM MECHANICAL TREATMENT OF SIMPLE SYSTEMS 11 hrs

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

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

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

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

3. APPROXIMATE METHODS AND MULTIELECTRON ATOMS 8 hrs

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

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

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

4.THEORY OF ANGULAR MOMENTUM 6 hrs

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

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

5. CHEMICAL BONDING 13 hrs

Diatomic molecules: Born-Oppenheimer approximation.

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

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

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

REFERENCES

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

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

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

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

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

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

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

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

2. MICROWAVE SPECTROSCOPY **8 hrs**

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

3. INFRARED SPECTROSCOPY **14 hrs**

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

4. RAMAN SPECTROSCOPY 8 hrs

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

5. ELECTRONIC SPECTROSCOPY 13 hrs

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

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

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

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

REFERENCES

1. Chemical Applications of Group Theory, F.A. Cotton, Wiley Eastern (2009).
2. Introduction to Molecular Spectroscopy, C.N. Banwell & M.McCash, TMH Pub (2010).
3. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (Int. Students Edition) (1988).
4. Molecular Spectroscopy, J.D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
5. Modern Spectroscopy, J.M. Hollas, John Wiley (2010).
6. Vibrational Spectroscopy, D.N. Sathyanarayana, New Age International (P) Ltd. (1996).
7. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, (2001).
8. A simple approach to group theory in chemistry. S. Swarnalakshmi, T Saroja and R M Ezhilarasi. Universities Press. ISBN: 9788173716232, 9788173716232

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

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

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1. ERRORS IN CHEMICAL ANALYSIS, STATISTICAL DATA TREATMENT AND EVALUATION (12+1) hrs

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

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

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

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

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

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

2. ACID – BASE TITRATIONS **8 hrs**

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

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

3. REDOX TITRATIONS **8 hrs**

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

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

4. PRECIPITATION TITRATIONS **4 hrs**

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

5. COMPLEXOMETRIC TITRATIONS **7 hrs**

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

6. GRAVIMETRIC ANALYSIS (4+1) hrs

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

7. KINETIC METHODS OF ANALYSIS (4+1) hrs

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

8. ABSORPTION AND EMISSION TECHNIQUES (6+1) hrs

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

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

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

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

9. THERMAL METHODS OF ANALYSIS 3 hrs

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

REFERENCES

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

PRACTICALS

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

QUALITATIVE ANALYSIS: 11 Units

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

REFERENCES

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

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

QUANTITATIVE ANALYSIS: **11 Units**

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

REFERENCES

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

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

I. QUALITATIVE ANALYSIS: 11 Units

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

REFERENCES

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

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

QUANTITATIVE ANALYSIS: **11 Units**

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

REFERENCES

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

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

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

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

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

SECOND SEMESTER
THEORY PAPERS

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

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

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

1. METAL – LIGAND BONDING (11+4) hrs

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

2. METAL – LIGAND EQUILIBRIA IN SOLUTION 8 hrs

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

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

4. VIBRATIONAL SPECTRA OF TRANSITION METAL COMPLEXES 4 hrs

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

5. ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES 12 hrs

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

6. MAGNETIC PROPERTIES OF METAL COMPLEXES (8+1) hrs

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

7. STRUCTURE AND BONDING IN SELECTED METAL COMPLEXES

(10+2) hrs

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

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

REFERENCES

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

3. Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, J.E. Huheey, E.A. Keiter and R.L. Keiter, Pearson Education Asia Pvt. Ltd. (2000).

4. Physical Methods in Inorganic Chemistry, Russell S. Drago, Litton Educational Publishing Inc. (1965).

5. Inorganic Chemistry, 7th Edition, M. Weller, J. Rourke, T. Overton and F. Armstrong, Oxford Univ. Press. (2018).

6. Inorganic Chemistry, G. Wulfsberg, Viva Books Pvt. Ltd. (2002).

7. Inorganic Chemistry, G.L. Miessler and Tarr, 5th edition, Pearson Education Ltd. (2014).

8. Coordination Chemistry, 2nd edition, D. Banerjea, Asian Books Pvt. Ltd. (2007).

9. Physical Inorganic Chemistry, S. F. A. Kettle Springer-Verlag GmbH(1996).

10. Inorganic Chemistry, 4th Edition, C. E. Housecraft and A. G. Sharpe, Pearson Education Ltd. (2012).

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

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

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

1. ADDITION REACTIONS 10 hrs

Addition to carbon-carbon multiple bonds: mechanisms of electrophilic addition reactions; regioselectivity and stereoselectivity; hydrogenation and hydroboration; Nucleophilic addition: Michael addition, mechanisms of formation of hydrates, acetals, oximes and hydrazones of carbonyl compounds, Wittig reaction.
Addition to carbon-hetero atom multiple bonds: mechanisms of metal hydride reduction of carbonyl compounds and nitriles. ***Addition of Grignard reagents and organolithium reagents to carbonyl compounds***

2. ALIPHATIC ELECTROPHILIC SUBSTITUTION 5 hrs

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

***Halogenation of aldehydes, ketones and acids, haloform reaction*.**

3. REARRANGEMENTS 15 hrs

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

4. PERICYCLIC REACTIONS 20 hrs

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

Molecular orbital symmetry; frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems; classification of pericyclic reactions. Theories to rationalize pericyclic reactions: Woodward-Hoffmann orbital symmetry correlation diagram, frontier molecular orbital approach (FMO), Woodward-Hoffmann rules, Hückel-Mobius (perturbation molecular orbital or transition state aromaticity) method.
Electrocyclic reactions: conrotatory and disrotatory modes; 4n, 4n+2 and allyl systems.
Cycloadditions: suprafacial and antarafacial additions, 4n and 4n+2 systems; [2+2] addition of ketenes, 1,3-dipolar cycloadditions and chelotropic reactions.
Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 1,3-, 1,5-, 3,3- and 2,3-sigmatropic rearrangements; Cope and Claisen rearrangements; Sommelet-Hauser rearrangement; Alder-Ene reaction.

5. FREE RADICAL REACTIONS AND PHOTOCHEMISTRY 10 hrs

(*Review/recall: Homolysis of bonds, photochemical excitation of molecules, Beer-Lambert's law, dissipation of energy - Jablonsky diagram*).
Generation of free radicals – thermolysis and photolysis of peroxides, peresters and azo compounds, hydrogen abstraction, chain process.
Free radical addition, substitution, elimination, rearrangement and electron transfer reactions. Use of free radicals in organic synthesis.
General principles of photochemistry: singlet and triplet states-differences in reactivity, photosensitisation; quantum efficiency, quantum and chemical yields.
Photochemical reactions: Norrish type I and type II cleavages, cis-trans isomerisation, di-π-methane rearrangement; Paterno-Buchi reaction; photoreduction of ketones; photochemistry of arenes.

REFERENCES

1. March's Advanced Organic Chemistry, Michael B. Smith and J. March, 6th Edn., John Wiley, (2007).
2. Advanced Organic Chemistry, Part A and B, F. A. Carey and J. Sundberg, 5th Edn., Plenum press, (2007).
3. Organic Chemistry, Paula Yurkanis Bruice, 7th Edn., Pearson Education, Inc., (2014).

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

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

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

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

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

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

10. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory, S. Sankararaman, Wiley VCH, 2005

11. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh, 4th Edn. New Age International Publishers,2019.

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

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

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

1 STATISTICAL THERMODYNAMICS (15+2) hrs

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

Maxwell Boltzmann statistics: assumptions, derivation of equation for fraction of molecules occupying a given energy range, partition function and its physical significance.

Bose-Einstein statistics: assumptions, ***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 – derivation of expressions for internal energy, heat capacity, free energy, chemical potential, pressure, entropy and equilibrium constant. Derivation of translational/rotational/vibrational/electronic partition functions. Sackur-Tetrode equation.

Evaluation of partition functions from spectral data, thermodynamic properties of molecules from partition functions.

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

2. CHEMICAL THERMODYNAMICS 15 hrs

Introduction –Review of thermodynamic laws and their significance.

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

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

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

3. NON-EQUILIBRIUM THERMODYNAMICS 8 hrs

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

4. REACTION KINETICS (16 + 2) hrs

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

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

Primary and secondary salt effects.

Kinetic and thermodynamic control of reactions.

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

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

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

5. KINETICS OF POLYMERIZATION 4 hrs

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

REFERENCES

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

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

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

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

1. UV AND VISIBLE SPECTROSCOPY 6 hrs

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

2. INFRARED SPECTROSCOPY 8 hrs

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

3. NMR SPECTROSCOPY 17 hrs

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

4. CARBON–13 NMR SPECTROSCOPY 7 hrs

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

5. ADVANCED NMR TECHNIQUES 5 hrs

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

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

6. MASS SPECTROMETRY 8 hrs

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

7. ELECTRON PARAMAGNETIC RESONANCE SPECTROSCOPY 6 hrs

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

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

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

REFERENCES

1. Physical methods in Inorganic chemistry, R.S. Drago, Affiliated East-West Press Pvt. Ltd., New Delhi (1965).
2. Infrared Spectra of Inorganic and co-ordination Compounds, K. Nakamoto, Wiley-Interscience, New York, (1970).
3. Vibrational spectroscopy: theory and Applications, D.N. Sathyanarayana, New-Age International Publishers, New Delhi (2000).
4. Electronic Absorption Spectroscopy and related techniques, D.N. Sathyanarayana, Universities Press, Bangalore, (2001).
5. Applications of absorption Spectroscopy to Organic Compounds, J.R. Dyer, Prentice – Hall, New Delhi, (1969).
6. Organic Spectroscopy, W. Kemp, ELBS London, (1975).
7. Spectrometric Identification of Organic Compounds, R.M. Silverstein and W.P. Webster, Wiley & Sons, (1999).
8. Organic Mass Spectroscopy, K.R. Dass and E.P. James, IBH New Delhi, (1976).

9. Mass Spectrometry of Organic Compounds, H. Budzkiewicz, Djerassi C. and D.H Williams, Holden-Day, New York, (1975).

10. Principles of Instrumental Analysis, D.A. Skoog, S.J. Holler, T.A. Nilman, 5th Edition, Saunders College Publishing, London, (1998).

11. Introduction to Spectroscopy, 5th Edition, Donald L. Pavia, Gary M. Lampman and George S. Kriz and James R. Vyvyan. Cengage Learning (2015).

12. Physical Methods for Chemists, R.S. Drago, 2nd Edition, Saunders College Publishing New York, (1992).

13. Mass Spectrometry – Analytical Chemistry By Open Learning -, R. Davies, M. Frearson and E. Prichard, John Wiley and Sons, New York, (1987).

14. Modern NMR techniques For Chemistry Research, Vol. 6, A.E. Derome, Oxford Pergamon Press, (1987).

15. Spectroscopic Methods in Organic Chemistry, 4th Edition, D.H. Williams and I. Fleming, Tata-McGraw Hill Publications, New Delhi, (1988).

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

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

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

1. SOLVENT EXTRACTION **7 hrs**

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

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

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

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

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

Nitrogen phosphorous detector, flame photometric detector, photoionization detector, Element specific plasma detectors.

4. LIQUID CHROMATOGRAPHY 19 hrs

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

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

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

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

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

5. Thin layer chromatography 2 hrs

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

6. Paper Chromatography **3 hrs**

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

REFERENCES

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

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

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

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

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

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

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

PRACTICAL PAPERS

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

Physical Chemistry Practical I

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

REFERENCES

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

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

Physical Chemistry Practical II

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

REFERENCES

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

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

Inorganic Compounds:

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

REFERENCES

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

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

II Organic Compounds:

1. 1. Preparation of benzanilide from benzophenone.
   2. Preparation of benzilic acid from benzoin.
   3. Preparation of anthranilic acid from phthalic acid
   4. Preparation of 2-iodoxybenzoic acid (IBX) from anthranilic acid and its application for oxidation of alcohol.
   5. Preparation of dibenzalacetone and reduction of carbonyl group.
   6. Application of *N*-bromosuccinimide (NBS) in allylic bromination.
   7. Preparation of an organic compound (one step preparation) by 2 or 3 different methods and comparison/evaluation of the methods with respect to the following parameters:
      (i) Ease of preparation, problems in handling chemicals, toxicity and flammability of chemicals
      (ii) Yield and cost effectiveness
      (iii) Product purity/quality
      (iv) Environmental compatibility (from the point of view of green chemistry)
   8. Any other experiments
   Characterization of the organic compounds (experiments 8–14) by: TLC, column liquid chromatography, fractional crystallization, UV, IR and NMR spectroscopic techniques.

REFERENCES

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

THIRD SEMESTER

THEORY PAPERS

Semester	III
Paper code	CH9122
Paper title	BIOLOGICAL CHEMISTRY
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

1. ESSENTIAL AND TRACE ELEMENTS IN BIOLOGICAL SYSTEMS (1 + 2) h

Role of metal ions in biological processes. Metal ion toxicity and detoxification - chelation therapy. Metal complexes in medicine: gold complexes and platinum complexes.

2. METAL ION STORAGE AND TRANSPORT (4 + 2) h

Ferritin, transferrin, ceruloplasmin, siderophores. ***Transport and storage of dioxygen: hemoglobin, myoglobin; phenomenon of cooperativity*****;** model systems (picket fence porphyrins), hemocyanin and hemerythrin.

3. TRANSPORT OF IONS ACROSS MEMBRANES 6 h

Thermodynamic treatment, active and passive transport, ionophores, Na^+/K^+ pump. Chemistry of vision and nerve conduction.

4. ELECTRON TRANSPORT PROTEINS 6 h

Rubredoxin, ferredoxins, cytochromes. Photosynthesis: chlorophyll, PS I, PS II, role of manganese-protein complex in electron transfer in photosynthesis. Nitrogen fixation: bacterial nitrogenase system. Biochemical importance of NO. Role of Ca in signal transduction.

5. ENZYMES 7 h

Mechanism of enzyme action. Examples of some typical enzyme mechanisms - chymotrypsin, lysozyme. Michaelis-Menten kinetics and derivation of the equation, modifications and extensions of Michaelis-Menten equation, significance of Michaelis-Menten parameters, graphical representation of data - Lineweaver-Burke and Eddie Hoftsee plots, enzyme inhibition kinetics (competitive, non-competetive, uncompetitive and mixed). Non-productive binding. Competing substrates. Reversibility – Haldane equation. Breakdown of Michaelis-Menten equation. Multisubstrate systems – brief description of different mechanisms (ordered, sequential and random).

6. METALLOENZYMES 9 h

Non-redox enzymes – carboxypeptidase A and carbonic anhydrase; redox enzymes - superoxide dismutase (mono and binuclear), peroxidase, catalase, cytochrome oxidase, Cyt P_{450}, ascorbic acid oxidase, alcohol dehydrogenase; cobalamine (coordination environment around the metal and mechanism of action of each enzyme to be discussed).

7. COENZYMES 7 h

Structure and typical reactions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid (one representative mechanism for each type of reaction).

8. BIOSYNTHESIS OF MACROMOLECULES 7 h

Pseudocycles - gluconeogenic pathway and its regulation. Biosynthesis of cholesterol and its regulation. Protein synthesis: genetic code, wobble hypothesis, five stages of translation – i) activation (including idea of regulation of aminoacyl t-RNA synthesis) ii) initiation process (including significance of Shine-Delgarno sequence) iii) elongation iv) termination and v) post translational modification.

9. BIOENERGETICS (3 + 2) h

Standard free energy change in biochemical reactions. Ways in which non-spontaneous reactions are overcome. ATP hydrolysis and synthesis, energy generation in mechano-chemical systems: muscle contraction.

10. BIOPOLYMER INTERACTIONS (2 + 2) h

Electrostatic charges, hydrophobic forces, dispersion forces. Various types of binding processes in biological systems.

REFERENCES:

1. Principles of Biochemistry, A. L. Lehninger, CBS, New Delhi (1993).
2. Biochemistry, L. Stryer, 2nd edition, CBS, New Delhi (1986).
3. Biochemistry, G. Zubay 4th Edition, WCB, Mcgraw Hill (1998).

4. Biochemistry, Voet and Voet, 2nd edition, John Wiley (1995).
5. Organic Chemistry, Paula Bruice (Pearson)
6. Bioinorganic chemistry, Asim K. Das, Books and Allied publishers (P) Ltd., Kolkata (2015).
7. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, Viva Books Pvt. Ltd., (1998).
8. Enzymes: Structure and Function, S Blackburn Marcel Dekker, (1976).
9. Enzymatic Reaction Mechanisms, C. Walsh, W. H. Freeman (1979).
10. Physical Chemistry with Applications to Biological Systems, Raymond Chang, McMillan (1977).
11. Bioorganic, Bioinorganic And Supramolecular Chemistry, P.S. Kalsi , J. P. Kalsi , Ashu Chaudhary, New Age International publishers, 2020.

Semester	III
Paper code	CH9222
Paper title	ORGANOMETALLIC CHEMISTRY AND INORGANIC REACTION MECHANISMS
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

1. ORGANOMETALLIC COMPOUNDS (5+2) h

Nomenclature of organometallic compounds; ***classification based on the hapticity of ligands and the polarity of C-M bond*****;** 18- electron rule, electron counting –covalent and ionic models; thermal, thermodynamic and kinetic stability and decomposition pathways; ***general methods of synthesis of organometallics of representative elements.***

2. ORGANOMETALLIC COMPOUNDS OF MAIN GROUP ELEMENTS 7 h

Group trends; structure and bonding in Li, Be, Mg and Al alkyls.

3. ORGANOMETALLIC COMPOUNDS OF TRANSITION METALS (12+2) h

Classification, structure, bonding, ***general methods of preparation and important classes of reactions of transition metal alkyls*****,** carbenes and carbynes; structure and bonding in transition metal complexes with dihapto to octahapto-donor ligands - alkene, allyl, 1,3-butadiene, cyclopentadienyl, ***arene, cycloheptatrienyl and cyclooctatetraenyl complexes***; metallocenes with special reference to ferrocene, cyclometallation and ring slippage reactions; activation of small molecules (CO and alkanes); isolobal analogy and its applications.

4. ORGANOMETALLIC COMPOUNDS IN ORGANIC SYNTHESIS (15+1) h

Green's rules; use of iron and chromium carbonyls in the synthesis of aromatic compounds; rhodium complexes in hydrogenation, hydroformylation, decarbonylation reactions; Monsanto acetic acid process; palladium complexes in thesynthesis of carbonyl compounds; Heck reaction; Wacker process; applications of zinc dialkyls, Grignard reagents, lithium alkyls, Gilman reagents (lithium dialkyl cuprates); organocadmium, organoselenium, organoaluminium, ***organosilicon, organotin and organomercurials in organic synthesis*****.** Zeigler-Natta catalysts (growth reaction, polymerization of olefins).

5. INORGANIC REACTION MECHANISMS (15+1) h

Kinetic lability and inertness, classification of metal ions based on lability; types of nucleophilic substitution reactions; kinetics and mechanism of nucleophilic substitution in square planar and octahedral complexes - trans effect; ligand field effects and reaction rates; reaction rates influenced by acids and bases, SN1CB mechanism; racemization and isomerization; mechanisms of redox reactions - outer sphere mechanism, Marcus equation for outer sphere cross reactions, excited state outer sphere electron transfer reactions, photochemical reactions of ruthenium complexes, inner sphere mechanism; oxidative addition and reductive elimination; migratory insertion; ***nucleophilic and electrophilic attack on coordinated ligands***; template reactions.

REFERENCES

1. Organometallic Chemistry, R.C. Mehrotra and A. Singh, Wiley Eastern (1991).
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, 6th edition, John Wiley & sons (2014).
3. Organometallics, Vol 1 & 2, M. Bochmann, Oxford Chemistry Primers, Oxford University Press (1994).
4. Organometallic Reagents in Synthesis, Paul R Jerkins, Oxford Chemistry Primers, Oxford University Press (1992).
5. Principles of Organic Synthesis, Sir Richard Norman and James M Coxon, 3rd edition, Chapman & Hall (1993).
6. Modern Synthetic Reactions, H.O. House and Benjamin (1972).
7. Reaction Mechanisms of Inorganic and Organometallic Systems, J. B. Jordan, Oxford University Press, 2nd edition (1998).
8. Inorganic Chemistry, G.L. Miessler, P. J. Fischer and D. A. Tarr, 5th edition, Pearson Education (2014).
9. Inorganic Chemistry, J. E. Huheey, E.A. Keiter and R.L. Keiter, 4th edition, Addison-Wesley (1993).
10. Basic Organometallic Chemistry: Concepts, Syntheses and Applications, B. D. Gupta and Anil J. Elias, 2nd edition, universities press (2013)

Semester	III
Paper code	CH9322
Paper title	ELECTROCHEMISTRY AND ELECTROANALYTICAL TECHNIQUES
Number of teaching hours per week	3
Total number of teaching hours per semester	45
Number of credits	3

1. THEORY OF STRONG ELECTROLYTES 8 h

Ionic atmosphere, Debye-Huckel theory of ion-ion interaction, Debye-Huckel equation in terms of activity coefficient, Debye-Huckel limiting law. Debye-Huckel equation for appreciable concentration, Huckel and Bronsted equation. Qualitative verification of the Debye-Huckel equation, ion association - ion pairs and triple ions and conductance minima.

2. ELECTRIFIED INTERFACE AND ELECTRODICS (10 + 2) h

The electrified interface: surface excess, interfacial tension and its determination, electrocapillary curves, thermodynamics of electrified interface — Lippmann equation, determination of the electrical capacitance of the interface, determination of surface excess. Structure of electrical double layer — Helmholtz-Perrin model, Gouy-Chapman diffuse charge model and Stern model. Electrodics: electron transfer under an interfacial electric field, equilibrium and exchange current densities, overpotential — dependence of current density on overpotential. Butler-Volmer equation and its special cases, the symmetry factor, influence of current density, pH and temperature on overvoltage. Tafel equation - derivation, Tafel plot.

Theories of overvoltage. Bubble formation as the slow process, combination of atoms as the slow process, ion discharge as the slow process and proton transfer as the slow process.

3. ELECTROANALYTICAL TECHNIQUES 25 h

3.1. ELECTROPHORESIS AND ELECTROCHROMATOGRAPHY (3+1) h

Important terms in electrophoresis, basis of electrophoretic separation. Expression for distance traveled on application of electrode potential. Role of buffer in electrophoresis.

Classical gel electrophoresis, high performance capillary electrophoresis – advantages. Instrumentation, sample injection. Comparison of classical and capillary electrophoresis.

Electroosmotic flow. Modes of electrophoresis: capillary gel electrophoresis, capillary isoelectric focusing, and capillary isotachophoresis.

***Capillary electrochromatography (basic principle). Micellar electrokinetic capillary electrophoresis*.**

3.2. ION SELECTIVE ELECTRODES (4+ 1) h

Potentiometry: electrodes used - metallic indicator electrodes (types with one example for each), metallic redox indicator electrodes, ion selective electrodes (ISE) - classification of ISE. Properties of ISE.

Glass membrane electrodes. Composition and structure of glass membrane. Hygroscopicity of glass membrane. Electrical conductance across the glass membrane. Membrane and boundary potential. Expression for E_b. Alkaline error. Crystalline membrane electrodes. Conductance of a crystalline membrane electrode.

Fluoride electrode. Electrodes based on silver salts. Liquid membrane electrode for Ca^{2+}. Molecular selective electrode systems. Gas sensing probe for CO_2.

Two types of gas sensing membrane materials, Biocatalytic membrane electrodes (two types of electrodes for the determination of BUN).

3.3. VOLTAMMETRIC TECHNIQUES (14+2) h

Polarization: ideal polarized and ideal non-polarized electrodes - sources of polarization. Reaction and concentration polarization. Mechanism of mass transport. The current response to applied potential (in terms of Fermi level and molecular orbitals) Faradaic and non-Faradaic currents. Charging and residual currents.

Polarography: Advantages of Hg over other solid electrodes. Types of mercury electrodes: DME, SMDE, HMDE and MFE. Instrumentation, potentiostat, function generator, three electrode system, and supporting electrolyte. Polarographic/IUPAC convention. Polarographic experiment. Polarographic parameters (diffusion current, half wave potential and their significance). Analysis of a polarogram. Effect of dissolved oxygen on electrochemical reduction process. Ilkovic equation (derivation). Quantitative and qualitative aspects of voltammetry: determination of concentration and standard state potentials. Determination of electrochemical reversibility and number of electrons. Effect of complex formation on polarographic waves. Determination of metal-ligand stoichiometry.

Potential excitation and response signal, and the corresponding voltammetric techniques: Linear scan polarography / voltammetry (LSP/V), staircase voltammetry (SV), normal pulse

(NPP/V), differential pulse (DPP/V), square wave (SWV) and cyclic voltammetry. Applications of polarography. Amperometric titrations at DME (all four types). Stripping voltammetry: cathodic, anodic and adsorption stripping voltammetry.

Cyclic voltammetry: excitation signal and current response in CV. Important parameters of CV. Instrumentation. Reversible, irreversible and quasireversible charge transfer and the diagnostic criteria. A cyclic voltammetric experiment - analysis of a cyclic voltammogram of potassium ferricyanide system. Cathodic and anodic processes. Working electrodes in voltammetry (glassy carbon, carbon paste, gold, platinum and modified electrodes). Coupled chemical reactions.

Coulometric methods of analysis: controlled-potential and controlled-current coulometry. Coulometric titrations, quantitative applications. Chronoamperometry and chronopotentiometry.

REFERENCES:

1. Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science; Amulya K.N. Reddy O'M. Bockris; Edition-, Kluwer Academic, New York (2010).
2. An introduction to Electrochemistry by Samuel Glasstone, Read Books Ltd, (2013), (e-book).
3. Principles of Instrumental Analysis, Skoog, Holler and Nieman, 7th edition, CENGAGE learning, Boston, USA (2016).
4. Analytical Chemistry Principles – John H Kennnedy, 2nd edition, Cengage India (2011).
5. Modern Analytical Chemistry David Harvey; 1st Edition, McGraw-Hill Higher Education, USA (2000).
6. Vogel’s Text book of quantitative chemical analysis, 6th edition, Pearson Education Limited (2007).
7. Electrochemical Methods Fundamentals and Applications, Allen J Bard and Larry R Faulkner, 2nd Edition, John Wiley and Sons, USA (2001).

Semester	III
Paper Code	CH9422
Paper Title	SOLID STATE CHEMISTRY
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

1. GENERAL METHODS OF SYNTHESIS OF SOLIDS (5 + 1) h

High temperature solid state synthesis; precursor methods; flux synthesis; combustion synthesis; chemiedouce (soft chemistry) methods; topotactic reactions; ***precipitation (including co-precipitation, and homogeneous precipitation),*** hydrothermal synthesis; sol-gel synthesis.

2. GEOMETRIC CRYSTALLOGRAPHY (12 + 2) h

Crystalline and amorphous states of matter (recall). Periodicity in crystals. ***Seven crystal systems with unit cell parameters and essential symmetry elements-axis of symmetry, plane of symmetry, centre of symmetry.*** Symmetry elements and symmetry operations. Pure rotation axis, roto-inversion, roto-reflection axes, screw axes, glide planes. Derivation of non-occurrence of five-fold rotation axis. Combination of symmetry operations – Euler's construction (inter-axial angles) and its application to the general formula of the type A.B = C. Plane lattices, space lattices, point groups and space groups. Number of point groups in each crystal system, crystal classes. Stereographic projections of the following point groups: 222, 32, 422, 622, 23, 432 (Supporting the interfacial angles Euler's construction); space group representation – Hermann-Maugin symbols of some selected space groups.

3. CRYSTAL STRUCTURES OF SOME REPRESENTATIVE SYSTEMS: 3 h

Olivines; corundum, ilmenite and $LiNbO_3$; garnets; K_2NiF_4 and Ruddlesden-Popper phases.

4. X-RAY DIFFRACTION (11 + 2) h

Generation of X-rays, ***Bragg's equation and Bragg's method, Miller indices, unit cell parameters.*** X-ray structural analysis of solid substances: powder diffraction pattern of primitive, face-centered and body centered cubic lattices, indexing of reflections – graphical method and trial and error method, identification of space groups from systematic absences (space group extinctions). The concept of reciprocal lattice and construction of Ewald's sphere, derivation of Bragg's law from reciprocal lattice, structure factor and its relation to intensity, intensities from atomic positions for BCC and FCC lattices. Phase problem - heavy atom (Patterson's) method, introduction to the principles of direct methods of phase determination. Electron density function and electron density maps.

5. ELECTRON AND NEUTRON DIFFRACTION 2 h

Principles of electron and neutron diffraction; comparison with X-ray diffraction and applications.

6. DEFECTS IN SOLIDS (3 + 1) h

Point defects – Schotky and Frenkel defects, ***colour centers and non-stoichiometric defects***. Line defects – edge dislocation and screw dislocation. Plane defects – grain boundary and stacking faults. Diffusion in solids, Fick's law.

7. PHASE TRANSITIONS IN SOLID 2 h

Definition and classification; first and second order phase transitions with examples.

8. ELECTRICAL AND MAGNETIC PROPERTIES OF SOLIDS (14 + 2) h

Band theory: electron in periodic potential; Bloch theorem; Kronig–Penny model (derivation excluded); band structure – extended, reduced and repeat zone representation; Brillouin zones; DOS plots; metals, semiconductors and insulators. Properties of metals – ***metal-metal junction, thermoelectricity.*** Semiconductors – intrinsic and extrinsic semiconductors, Fermi levels of intrinsic, n-type and p-type semiconductors, electrons and holes, ***metal-semiconductor junction, p-n junction.*** Insulators – dielectric properties, piezoelectric effect, ferroelectricity, ferroelectric transitions in $BaTiO_3$, ionic conduction, electric breakdown. Magnetic properties of solids – paramagnetism, diamagnetism, ferromagnetism and anti-ferro magnetism – M vs H and χ vs T curves.

REFERENCES :

1. Introduction to solids - L.V. Azaroff, Tata-McGraw Hill Publishing Company, New Delhi (1977).

2. Fundamentals of Crystallography - edited by C. Giacovazzo, International Union of Crystallography, Oxford University Press (2002).

3. Elements of X-Ray Diffraction- B. D. Cullity, S.R. stock, Pearson Education Ltd. (2014).

4. The Basics of Crystallography and Diffraction - C. Hammond, International Union of Crystallography, Oxford University press (2001).

5. Solid State Chemistry and its Applications - A.R. West, John Wiley and Sons (1984).

6. A Basic Course in Crystallography - J. Tareen and TRN Kutty, Universities Press (2001).

7. Principles of the Solid State - H.V. Keer, Wiley Eastern Ltd. (1993).

8. Solid State Chemistry - D.K. Chakraborty, New Age International Publishers (2000).

9. An Introduction to X-Ray Crystallography - M.M. Wolfson, Cambridge University Press (1997).

10. Crystal Structure Analysis for Chemists and Biologists, J.P. Glusker, M. Levis and M. Ross, Wiley-VCH (1994).

11. X-Ray Structure Determination – G.H. Stout and L.H. Jensen, McMillan Publishing Co, (1968).

12. Solid State Physics- S. L. Gupta and V. Kumar, K. Nath and Co, Meerut, (2003).

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

1. CHEMISTRY AND SOCIETY **2 h**

An introduction of the impact of chemistry on society.

2. MOLECULAR GASTRONOMY **5 h**

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

3. FORENSIC CHEMISTRY **5 h**

What is forensic science? An idea of the analytical techniques used: a) Atomic Spectroscopy b) Microspectrophotometry c) Electrophoresis d) Microscopy e) Chromatography f) Immunoassays. Analysis of Forensic Samples – a) Drug Analysis b) Combustion & Arson c) Inks, Paints, & Pigments d) Polymers & Fibers

4. MOLECULAR PROCESSES **3 h**

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

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

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

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

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

REFERENCES:

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

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

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

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

Three ways of starting a chemical reaction in kitchen:

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

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

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

2. METHODS OF COOKING **5 hrs**

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

3. CHEMISTRY OF COOKING **7 hrs**

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

4. GRAINS, BREAD AND LEAVENING **7 hrs**

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

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

5. AMATEUR TO FOOD SCIENTIST **5 hrs**

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

References

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

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

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

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

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

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

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

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

THIRD SEMESTER

PRACTICAL PAPERS

Semester	III
Paper Code	CH9P1
Paper Title	Practical: APPLIED ANALYSIS - I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Inorganic Chemistry **11 sessions**

1. Non-aqueous titration (1 session)
2. Analysis of alloy (Steel - Cr, Fe or other alloys) (2 sessions)
3. Analysis of soil (Cation exchange capacity and organic matter) (2 sessions)
4. Ion exchange Chromatography (Zn & Cd) (2 sessions)
5. Solvent extraction (Estimation of Fe III) (1 session)
6. Determination of metal to ligand ratio by Job's method (1 session)
7. Preparation of Ionic liquids (1 session)
8. Preparation of graphite- intercalated compounds (RBPT) (1 session)

REFERENCES:

1. Text book of Quantitative Inorganic Analysis by A.I. Vogel, ELBS (1978).
2. Advanced Physicochemical Experiments by Rose, Isaac Pitman (1964).
3. Methods of Soil Analysis Part I & II, C.A. Black et al, American Society of Agronomy, Inc. (1965).
4. Analytical Chemistry-An introduction; Skoog, West, Holler and Crouch; seventh edition Saunders College Publishing, (1999).
5. Experiments in Environmental chemistry, P.D. Vowels and D.W. Connel, Pergamon (1980).

Semester	III
Paper Code	CH9P2
Paper Title	Practical: APPLIED ANALYSIS - II
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Experiments in Biochemistry **11 sessions**

1. Estimation of rancidity in a sample of butter.
2. Estimation of BOD and COD of a sample.
3. Extraction of caffeine from tea leaves and characterization using IR, NMR and Mass spectrometer.
4. Estimation of glucose in serum.
5. Estimation of sulpha drug using spectrophotometer.
6. Estimation of RNA using spectrophotometer.
7. Estimation of cholesterol in serum.
8. Gel electrophoresis- separation of proteins.
9. Agarose gel electrophoresis-separation of RNA/DNA
10. Separation, purification and characterization of protein from plant sample
11. Any other suitable experiments.

REFERENCES:

1. Textbook of Practical Organic Chemistry, A I Vogel, ELBS (1973).
2. Practical Clinical Biochemistry, H. Varley, 4th edition, CBS Indian edition (1988).
3. An Introduction to Practical Biochemistry, David Plummer, Tata McGraw Hill (1979).
4. Laboratory Manual in Biochemistry, J. Jayaraman, Wiley Eastern (1981).
5. Chromatography, C.G. Sharma Krishna Prakashana Media (1997).

Semester	III
Paper Code	CH9P3
Paper Title	Practical: ADVANCED METHODS OF ANALYSIS I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Atomic Absorption Spectroscopy

1. Estimation of iron in a given sample using AAS
2. Estimation of an alloy (Cu, Zn and Pb) using AAS

Chromatography

3. Estimation of halide ions in a given mixture using ion chromatography
4. Estimation of alkali metal ions in a mixture using ion chromatography
5. Separation and identification of organic compounds using GC
6. Estimation of caffeine using HPLC

Thermogravimetric Analysis

7. Thermal analysis (TGA/DTA) of a given sample

Fluorescence Spectroscopy

8. Estimation of a dye by fluorescence spectroscopy

UV-Visible Spectroscopy

9. Estimation of bandgap of a solid
10. Kinetic studies using UV-Vis spectroscopy
11. Any other suitable experiment (GC/LC-MS etc.)

REFERENCES:

1. Vogel, Arthur I: A Text book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others), 5 th Ed. 1986.
2. Willard, Hobart H. et al., Instrumental Methods of Analysis, 7 th Ed. Wardsworth Publishing Company, 1988.
3. Christian, Gary D; Analytical Chemistry, 6 th Ed. John Wiley & Sons, 2004.
4. Khopkar, S.M. Basic Concepts of Analytical Chemistry, 2009.
5. Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, 1998.

Semester	III
Paper Code	CH9P4
Paper Title	Practical: ADVANCED METHODS OF ANALYSIS II
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Flame Photometry

1. Estimation of sodium/potassium/lithium by flame photometer.
2. Estimation of alkali metals in a given mixture by flame photometer.

Spectrophotometry

3. Estimation of caffeine in a given sample using UV spectrophotometer.
4. Estimation of Ni in tea powder.
5. Estimation of chloride in pharmaceutical products.
6. Estimation of mixture of Mn and Cr.

Electroanalytical Methods

7. Estimation of copper by potentiometry.
8. Estimation of sulphides in water sample by potentiometry
9. Estimation of a mixture of chloride and iodide by potentiometry.
10. Studying electrochemically reversible ferrocyanide-ferricyanide system using cyclic voltammetry.

REFERENCES:

1. Vogel, A.I. A text book of Quantitative Analysis, ELBS 1986.

2. Khosla, B. D.,Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co. (2011).

3. Garland, C. W., Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry, 8th Ed, McGraw-Hill: New York (2003).

4. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co., (2003).

FOURTH SEMESTER

THEORY PAPERS

Semester	IV
Paper Code	CH0121
Paper Title	APPLIED ANALYSIS
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

1. BIOPOLYMERS **3 h**

Determination of size, shape and molecular weight by sedimentation, diffusion and viscosity methods.

2. PROTEIN ANALYSIS **(13 + 2) h**

Protein purification: protein isolation, solubility of proteins, ***chromatographic separations***, ***electrophoresis and centrifugation***. ***Analysis and determination of protein structure: primary structure***, protein modification, secondary structure, globular and fibrous proteins, tertiary structure, quaternary structure. Techniques for study of biomolecules (principle and interpretation of data to characterize the biomolecule) – mass spectrometry (MALDI/ SELDI), confocal microscopy, microarrays, flow cytometry, microcalorimetry, differential scanning calorimetry, ELISA, RIA, FACS, Northern, Southern, Western blots, NMR, electrophoresis, CD, ORD, X-Ray crystallography.

3. NUCLEIC ACID ANALYSIS **(3 + 2) h**

Analysis and determination of structure of nucleic acids: ***primary structure, secondary structures, denaturation, renaturation, tertiary structure***. Chemical synthesis of polynucleotides. Recombinant DNA: cloning, DNA libraries, PCR and recombinant DNA technology. A brief account of the application of recombinant technology in different disciplines - industry, medicine and forensics.

4. FOOD ANALYSIS **(4 + 2) h**

Analysis of common adulterants in foods. Food additives: monosodium glutamate. Food preservatives: sodium benzoate, sodium sulphite. Milk and milk products-alcohol test, fermentation test, dye reduction tests (methylene blue and resazurin), phosphatase test for pasteurisation, ***estimation of added water in milk***. Beverages- caffeine and chicory in coffee, methanol in alcoholic drinks. Estimation of saccharin, coal tar dyes and aflatoxins in foods. Pesticide analysis in food products: phospho- and chloro- pesticides.

5. ANALYSIS OF DRUGS AND POISONS **(4 + 2) h**

***Classification of drugs, characterisation of common drugs: analgesics - aspirin; expectorants – benadryl; vitamins - vitamin C; sedatives - diazepam; antibiotics - penicillin, chloramphenicol; cardiovascular – sorbitrate*. ** Determination of barbiturate drugs (phenobarbital) in drug samples, and its clinical significance. Analysis of snake venom poison: phospholipases, hyaluronidase, toxic peptides.

6. CLINICAL CHEMISTRY **4 h**

Blood analysis: serum electrolytes, serum proteins, blood glucose, blood urea nitrogen, uric acid, and blood gas analysis. Enzyme analysis: assay of alkaline phosphatase, assay of Serum glutamic oxaloacetic transaminase and Serum glutamic pyruvic transaminase and their clinical significance, isoenzymes of lactate dehydrogenase, aldolase. Metal deficiency and disease: estimation of calcium, iron, and copper.

7. LIPID ANALYSIS **3 h**

Edible oils - qualitative tests for purity, estimation of rancidity, tests for common adulterants in edible oils.

8. POLLUTION ANALYSIS **10 h**

Air pollution: principles and methods of sampling; a survey of reactions and methods involved in the determination of carbon monoxide, sulphur oxides, nitrogen oxides, hydrocarbons and particulates. Tolerance limits. Fuel Analysis and emissions: ultimate and proximate analysis of coal, quality of liquid fuels - octane number, cetane number and carbon residue.

Water pollution: objectives of analysis; parameters of analysis: colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen; heavy metal pollution: public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental techniques for the analysis of heavy metals in aqueous systems.

9. SOIL ANALYSIS 4 h

Chemical properties of soil - types of soil colloids, types of clays and their swelling and adsorption properties, cation exchange capacity and its determination. Acid soils - types of soil acidity, liming, measurement of pH and conductivity of soil. Saline and alkaline soils. Analysis of major constituents of soil - organic matter, nitrogen, sulphur, sodium, potassium and calcium.

10. RADIOACTIVE POLLUTION 4 h

Detection and monitoring of radioactive pollutants; methods for the safe disposal of radioactive waste. Dosimetry. Advantages and restrictions of radiotracer experiments, safety aspects.

REFERENCES:

1. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern (1993).
2. Biochemistry, Voet and Voet, 2nd edition, John Wiley (1995).
3. Experiments in Environmental Chemistry, P.D. Vowels and D.W. Connel, Pergamon (1980).
4. Handbook on Air Pollution, Stern, APHA (1980)
5. Principles of Instrumental Analysis, D.A. Skoog and West. Saunders College (1980).
6. Food Analysis, A. G. Woodman, McGraw Hill (1971).
7. Milk and Milk Products, C.H. Eckles, W.B. Combs and H. Macy, Tata McGraw Hill (1976).

8. The Essentials of Forensic Medicine and Toxicology, K.S. Narayan Reddy, Suguna Devi, Hyderabad (2002).
9. Practical Clinical Biochemistry, H. Varley, 4th edition [CBS] Indian edition (1988).
10. Separation Techniques in Chemistry and Biochemistry, Roy Keller, Marcel. Dekker (1967).
11. Methods of Soil Analysis Part I & II, C.A. Black et al (Edition), American Society of Agronomy (1965).

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

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