KUMAUN UNIVERSITY NAINITAL

CBCS BASED SYLLABUS FOR FOUR SEMESTER (TWO YEAR)
M.Sc. DEGREE IN CHEMISTRY

Effective from academic year 2020-2021

CHEMISTRY
COURSE STRUCTURE
CBCS pattern

Semester I

Course	Core Course and Basic/Supporting	Credit
CHEM 101	Inorganic Chemistry -I	4
CHEM 102	Organic Chemistry - I	4
CHEM 103	Physical Chemistry - I	4
CHEM 104	Group Theory and Instrumentation Chemistry-1	4
CHEM Lab1	Practical-1(CHEM 101 and CHEM 102)	2 + 2
Basic/supporting courses	a. Biology for Chemist (for Mathematics student) b. Mathematics for Chemist (for Biology student)	2 2

Total Number of Credits for Semester I = 22 (18 Theory + 4 Practical)

Semester II

Course	Core Course	Credit
CHEM 201	Inorganic Chemistry -II	4
CHEM 202	Organic Chemistry - II	4
CHEM 203	Physical Chemistry - II	4
CHEM 204	Spectroscopic Techniques -I	4
CHEMLab2	Practical – 2 (CHEM 202 and CHEM 203)	2 + 2

Total Number of Credits for Semester II = 20 (16 Theory + 4 Practical)

Semester III

Course	Core Course	Credit
CHEM 301	Solid State Chemistry	4
CHEM 302	Spectroscopic Techniques- II	4
CHEM 303	Chemistry for Biological System	4
CHEM 304	Inter Disciplinary Topics in Chemistry	4
CHEM 305	Photo Chemistry and Allied Chemistry	4
CHEMLab3	Practical – 3(Inorganic/ Physical Chemistry)	2 + 2

Total Number of Credits for Semester III = 24 (20 Theory + 4 Practical)

Semester IV

Course	Elective Course	Credit
CHEM 40(I)	Two Elective Courses in Inorganic Chemistry group	4 + 4
CHEM 40(O)	Two Elective Courses in Organic Chemistry group	4 + 4
CHEM 40(P)	Two Elective Courses in Physical Chemistry group	4 + 4
CHEMLab4	Laboratory course/ Project work	4
Project/Dissertation		2

Dissertation/Project work; each student of IV semester shall be assigned a topic for project work by an Advisor. The students will work in the research lab of his/her Advisor and shall

assist the research scholar working in the lab, learn operation of lab techniques practically and shall submit a project report before the commencement of IV semester practical examination. The Project work/dissertation will be evaluated by the external examiner.

Total Number of Credits for Semester IV = 14 (08 Theory + 4 Practical + 2 project work)

Grand Total Credits: 64 (Core courses) + 2 (Basic course), 12 (Elective course) and 2 (Project work) = 80

Elective papers: Students will have to elect any two papers from one of the following groups.

Inorganic Chemistry; **Group-1**

CHEM 40(I_1): General and Organometallic Chemistry
CHEM 40(I_2): Inorganic polymer and supramolecular Chemistry
CHEM 40(I_3): Photo Inorganic Chemistry
CHEM 40(I_4): Environmental Chemistry

Organic Chemistry; **Group-2**

CHEM 40(O_1): Organic Synthesis
CHEM 40(O_2): Chemistry of Natural Products and Heterocyclic Compounds
CHEM 40(O_3): Medicinal Chemistry

Physical Chemistry; **Group-3**

CHEM 40(P_1): Physical organic and Quantum Chemistry
CHEM 40(P_2): Advanced Chemical Dynamics, Thermodynamics
CHEM 40(P_3): Advanced Photochemistry and Nuclear Chemistry

Note: ***In the IVth Semester, the candidate shall have to opt minimum of two elective papers of a particular specialization e.g. Inorganic/Organic/Physical. The candidate shall not be allowed to opt papers from different specializations, i.e. two elective papers are to be taken positively from one specialization, e.g. one from Inorganic and one from organic shall not be allowed, similarly other combinations shall not be allowed. The candidate shall have to do a minimum of five lab experiments from the list of the experiments given in the syllabus. He/ She will have to do a Project. The topic of the project shall be allotted to him/her by the Project Advisor. Two credit points are allotted for the project work and a report has to be submitted to the head of the department before the commencement of practical examination. The project report shall be evaluated by the external examiner on the day of practical examination.***

Pattern of examination

A. Theory

Each theory paper shall be of 03 hours and will consist of two sections, A and B.
***Section A**: (Short answers type with reasoning); 40% of the total marks (30 marks, seven questions of six marks each, any five have to be attempted).*
***Section C**: (Long answers type); 60 % of the total marks, (45 marks, all the three questions have to be attempted, internal choice will be given. Each question carries 15 marks).*

B. Internal assessment

For each theory paper, an internal assignment (in the form of class test and or assignments including classroom attendance) of 25 marks for each paper shall be conducted during each semester. The evaluated answer sheets/assignments have to be submitted to the Head of the Department/ Principal along with one copy of award list. The marks obtained have to be uploaded onto the University examination portal and the print out of the award list from portal have to be submitted to the Controller Examination.

C. Practical

The practical work of the students has to be evaluated periodically. The internal assessments (in the form of lab test, lab record, internal evaluation, assignment/home assignment and attendance) of total 15 marks for each semester shall be conducted during the semester. A minimum of 12 experiments covering all the kinds of exercises have to be conducted during a semester. In each semester, practical examination of 75 marks has to conducted by two examiners (External and internal) having duration of time 8 hours. The total number of students to be examined per batch should not be more than sixty. One copy of award list of the practical examination along with attendance has to be submitted to the Head of the Department/ Principal. The marks obtained have to be uploaded onto the University examination portal and the print out of the award list from portal have to be submitted to the Controller Examination.

SEMESTER I Paper I

Inorganic Chemistry-1

S.No.	Contents	Contact Hours/ Lecturer
1	**(a)Stereochemistry and Bonding in Main Group Compounds** Origin of VSEPR theory and its significance in main group structural chemistry, structure of SF_4,TeF_5^-,BrF_3, ICl_2^-,ICl_4^-, OF_2, OSF_4 , XeF_6 and IF_7,dπ-pπ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules. **(b) Compounds of Boron, Carbon and Nitrogen with Metals :**Metal borides, carbides and nitrides: preparation, properties, structures and application.	12 Lectures
2	**Metal-Ligand Equilibria in Solution:** Concept of thermodynamic and kinetic stabilities of metal complexes. Stepwise and overall formation constants and their correlations, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry	9 Lectures
3	**Metal π-Acid Complexes:** Metal carbonyls: structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidations, important reactions of metal carbonyls; preparation, bonding**,** structure and important reactions of transition metal nitrosyls, complexes of dinitrogen, dioxygen and tertiary phosphine.	9 Lectures
4	**Cluster Compounds:** Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and metalhalide clusters. Clusters with metal-metal multiple bonds.	9 Lectures
5	**Polyoxometalates:** Isopoly and heteropoly acids and salts (or anions) with special reference to vanadium, molybdenum and tungsten. Nomenclature, classification, preparation and structural aspects of poly acids and polyanions.	9 Lectures

Books Recommended:

i. F. A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advance Inorganic Chemistry, Sixth Edition, John Wiley & Sons , New York, 2003.

ii. J. D. Lee, Concise Inorganic Chemistry, Fifth Edition, Wiley India, 2012.

iii. Atkins, Overton, Rourke, Weller and Armstrong, Inorganic Chemistry, Oxford University Press.

iv. J. E. Huheey, E. A Keiter and R. L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, Fourth Edition, Pearson Education, 2003.
v. W. W. Porterfield, Inorganic Chemistry: A Unified Approach, Elsevier.
vi. G. Wulfsberg, Inorganic Chemistry, Viva Books.
vii. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, Pearson Education.

SEMESTER I Paper II

Organic Chemistry-1

S.No.	Contents	Contact Hours/ Lectures
1	**Nature of Bonding in Organic Molecules:** Delocalized chemical bonding conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromatcity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Hückel's rule, energy level of π - molecular orbitals, annulenes, antiaromaticity, ψ-aromaticity, homo-aromaticity, PMO approach. Bond weaker than covalent bond, addition compounds, crown ether complexes andcryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.	6 Lectures
2	**Stereochemistry:** Molecular symmetry and chirality: symmetry operations and symmetry elements, point group classification and symmetry number. Stereoisomerism: Classification, racemic modification, molecules with one, two or more chiral centres. Configuration, nomenclature, D, L, R, S and E, Z nomenclature. Axial and planar chirality and helicity (P & M); stereochemistry and configurations of allenes, spiranes, alkylidene, cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes. Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature, stereogenicity, cyclostereoisomerism; configurations, conformations and stability of cyclohexanes, (mono-, di- and tri-substituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalines, decalols, decalones.. Assymetric induction; Cram's, Prelog's and Horeaus rules. Dynamic stereochemistry (cyclic and acyclic). Qualitative correlation between confirmation and reactivity- Curtin-Hammitt principle. Stereochemistry of compounds containing N, S and P. chirogenicity, pseudoasymmetry and stereogeniccentre. Stereoselectivity, stereospecificity, regioselectivity and chemoselectivity. Enantiomeric and diasteriomeric excess.	12 Lectures
3	**PericyclicReactions:** Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-	10 Lectures

	Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motions, 4n, 4n+2 and allyl system. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, 3,3- and 5,5 sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements. Fluxional tautomerism, Ene reaction.	
4	**Aliphatic Nucleophilic Substitution:** The S_N^2, S_N^1, mixed S_N^1 and S_N^2, S_N^i and SET mechanisms. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity. Neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system.	6 Lectures
5	**Aromatic Nucleophilic Substitution:** The S_N Ar, S_N^1, benzyne and S_N^1 mechanism. Reactivity-effect of substrate structure leaving group and attacking nucleophile. The Von-Richter, Sommelet-Hauser and Smiles rearrangements.	6 Lectures
6	**Mechanism of Carbocation Rearrangement Reactions:** Pinacol-Pinacolone rearrangement, Wagner-Meerwein rearrangement, Benzilic acid rearrangement, Allylic rearrangement, Hofman reaction, Schmidt reaction, Baeyer-Villiger oxidation, Cumene-Hydroperoxide rearrangement, Curtius rearrangements, Lossen rearrangement, Dakin reaction. Application of NMR Spectroscopy in detection of carbocations	8 Lectures

BOOKS SUGGESTED:

i. Jerry March, Advanced Organic Chemistry Reactions, Mechanism and Structure, John Wiley.
ii. R. T. Morrison and R. N. Boyd, Organic Chemistry, Prentice Hall.
iii. C. K. Ingold, Structure and Mechanism in Organic Chemistry, Cornell University Press.
iv. S. M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry, Macmillan.
v. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International
vi. P. S. Kalsi, Stereochemistry of Organic Compounds, New Age International.
vii. S. M. Mukherjee, Pericyclic Reactions, Macmillan, India.
viii. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Plenum.
ix. Benjamin , Modern Organic Reactions, HO House.
x. Ernest L. Eliel and Samuel H. Wilen, Stereochemistry of Organic Compounds, Wiley India
xi. Ernest L. Eliel, Stereochemistry of Carbon Compounds. Tata McGraw Hill.

SEMESTER I Paper III

Physical Chemistry-1

S.No.	Contents	Contact Hours/ Lectures
1	**Thermodynamics:** Laws of thermodynamics: Fundamental concepts, state and path dependent functions, determination of work done, enthalpy change, and internal energy change in reversible and irreversible expansion and compression, entropy and its calculations, residual entropy, zero, first, second, third law of thermodynamics and their applications. Nerst theorem, spontaneity, free energy and its calculation, properties of Helmholtz free energy and Gibb's free energy, thermodynamic equilibria and free energy functions, Clausius-Claypeyron equation, chemical potential and entropies. Partial molar properties; partial molar free energy, partial molar volume and chemical potential and their significance, Gibbs-Duhem equation, methods of determination of partial molar quantities, Concept of fugacity and its determination, chemical potential and fugacity, thermodynamic functions of mixing. Non-ideal systems; Excess functions for non-ideal solutions, activity, activity coefficient, Debye-Hückel theory for activity coefficient of electrolytic solutions, determination of activity coefficients, ionic strength, application of phase rule to three component systems.	24 Lectures
2	**Chemical Dynamics :**Third and general order reactions, Experimental methods for kinetic studies, *viz*; conductometric, potentiometric and spectrophotometeric methods, effect of temperature on rate of reaction, Arrhenius equation. Chemical molecular dynamics: Collision theory of reaction rates, steric factor, activated complex theory, comparison of collision and activated complex theories, ionic reactions, kinetic salt effects, steady state concept, kinetic and thermodynamic control of reactions. Ki netics of gaseous reactions on solid surface, unimolecular and bimolecular surface reactions, kinetics of condensation and addition polymerization reactions, mechanism of H_2-Br_2, H_2-Cl_2 reactions, decomposition of the following compounds : acetaldehyde, ozone and H_2O_2.	24 Lectures

Books Recommended:

i. B. R. Puri, L. R. Sharma and M. S. Pathnia, Physical Chemistry, Milestone Publisher & Distributors, New Delhi.
ii. K. L. Kapoor, Physical Chemistry. Macmillan Publishers India Limited.
iii. K. J. Laidler,Kinetics, Pearson Education India.

SEMESTER I Paper IV

Group Theory and Instrumentation Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Symmetry and Group Theory in Chemistry:** Symmetry elements and symmetry operations, definitions of group and subgroup and their characteristics, relation between orders of and subgroup and their characteristics, relation between orders of a finite group and its subgroup. Conjugacy relation and classes of symmetry operations, point symmetry (or group) and its classification, Schonfliess symbols, representation of group by matrices (representation for the C_n, C_{nv}, C_{nh} etc. groups to be worked out explicity), products of symmetry operations. Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use in spectroscopy.	16 Lectures
2	**X-ray Diffraction Methods:** Bragg condition, Miller indices, Laue's method, Bragg's method, Debye- Scherrer method of X-ray structural analysis of crystals. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules. Ramchandran diagram. General Introduction of Electron Diffraction: Scattering intensity vs scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules.	12 Lectures
3	**Chromatographic methods:** Principle, instrumentation and applications of gas and liquid chromatography. Principle and application of TLC, paper, column and HPLC. Ion Exchange chromatography: Cationic, anionic exchangers and their applications. Gas Chromatography: Theory of gas chromatography, parts of gas chromatograph, detectors (TCD, FID, ECD), Van-Deemter equation (no derivation), concept about HEPT- plate theory and rate theory. Applications.	15 Lectures
4	**Radio Analytical Methods:** Basic principles and types of measuring instrument, isotope dilution techniques- principle of operations and uses. Applications.	5 Lectures

Books Recommended

i. F.A. Cotton, Chemical Application of Group Theory, Wiley.

ii. D. C. Harris, Bertolucci, Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy, Dover Publications, New York.

iii. P. K. Bhattacharya, Group Theory and its Chemical Applications, Himalaya Publishing House, Mumbai.

iv. Gurdeep Raj, Ajay Bhagi and Vinod Jain, Group Theory and Symmetry in Chemistry, Krishna Prakashan Media (P) Ltd., Meerut.

SEMESTER I Paper V

Biology for Chemist (For students who had Mathematics at B. Sc. level)

S.No.	Contents **Section A**	Contact Hours/ Lectures
1	**Cell as Unit of Lite:** The cell theory; prokaryotic and eukaryotic and eukaryotic cells; cell size and shape; Eukaryotic cell components	12 Lectures
2	**Cell Organelles:** Mitochondria: Structure, marker enzymes, composition; function. Chloroplast: Structure, marker enzymes, composition; semiautonomous nature, chloroplast DNA. ER, Golgi body and Lysos omes: Structures and roles of ER, Golgibody and lysosomes Nucleus: Nuclear Envelope- structure of nuclear pore complex; chromatin; molecular organization, DNA packaging in eukaryotes, euchromatin and heterochromatin, nucleolus and ribosome structure (brief). Nacleoside and Nacloeotides and DNA structure	12 Lectures
3	**Cell Membrane and Cell Wall:** The functions of membranes; Models of membrane structure; faces of the membrane, selective permeability of permeability of the membranes; cell wall	12 Lectures
4	**Metabolism:** Introduction, basal metabolic rate (BMR), Carbohydrate protein and lipid metabolism, cell respiration, amaerabic respiration, aerobic respiration, formation of acetal COA, citric acid cycle, electron transport system, adenosinetri phosphate, mechanism of ATP generation	

Books Recommended:

i. P. H. Raven, Biology, Tata MacGraw Hill.
ii. P. Sheeler, Cell and Molecular Biology, John Wiley.
iii. N. A. Campbell, Biology Pearson.
iv. L. Styer, Biochemistry, Freeman & Co.
v. Outlines of biochemistry. Fourth edition (Conn, Eric E.; Stumpf, P. K.). Wiley India Pvt. Limited

SEMESTER I Paper V

Mathematics for Chemist (for students who had bio subjects at B. Sc. level)

S.No.	Contents **Section B**	Contact Hours/ Lectures
1	**Mathematical Functions:** Polynomial expression, exponential function, trigonometrically function. inverse trigonometrically function. Logarithms and anti logarithms	08 Lectures
2	**Curve Sketching/Graph:** Inclination of a line and the slope of a line, General equation of straight line, slope-intercept form, slope point form. Two point form, Intercept form, Parallel and perpendicular lines	08 Lectures
3	**Differentiation:** Differentiation formulas, Concept of maximum and minimum, Rules of finding maxima and minima, Partial differentiation, Euler reciprocal relation, exact and in exact differentials, Chain rule for partial differential	08 Lectures
4	**Integration:** Methods of integrations, substitution, partial function, by parts, successive, reduction, integration formulas including concept of limit	09 Lectures
5	**Fundamentals of Mathematical Relations**: Permutations and Combination, Probability, vectors mathematical relations, Vectors, Matrices, Determinants, Complex number, Series, Stirling approximation, Roots of quadratic equation. Methods of solving equation. Coordinate systems in three dimensions (Cartesian, spherical and polar).	15 Lectures

Books Recommended:

i. D.A. McQuarrie, Mathematics for physical Chemistry University Science Books.
ii. R. Mortimer, Mathematics for Physical Chemistry, 3rd Ed. Elsevier.
iii. E. Steiner, The Chemical Maths Books, Oxford University Press.

Laboratory Course **08 hrs**

A: Inorganic Chemistry

(I) Qualitative Analysis 18

Qualitative analysis of mixtures of salts containing not more than eight radicals including:

(i) Rare-earth element salts (two rare element ions)
(ii) Interfering radicals
(iii) Other anions, which have not been done in under graduate practical.
(iv) Insolubles and simple salts

(II) Preparations

Preparation of selected inorganic compounds such as: 12

1. $[Ni(dmg)_2]$
2. $[Cu(NH_3)_4]SO_4.H_2O$
3. Cis-$K[Cr(C_2O_4)_2(H_2O)_2]$
4. $Na[Cr(NH_3)_2(SCN)_4]$
5. $[Mn(acac)_3$]
6. $K_3[Fe(C_2O_4)_3]$
7. Prussian Blue, Tumbull's Blue
8. $Co[NH_3)_6][Co(NO_2)_6]$
9. Cis-$[Co(trien)(NO_2)_2]Cl.H_2O$
10. Hg $[Co(SCN)_4]$
11. $[Co(py)_2Cl_2]$
12. $[Ni(NH_3)_6]Cl_2$

OR

Quantitative estimation of metal ions by complexometric titration, direct and / or back titration, use of masking agents. 12

B. Organic Chemistry

1. Quantitative Analysis 18

i. Determination of the percentage of number of hydroxyl groups in an organic compound by acetylation method.

ii. Estimation of amines/ phenols using bromate-bromide solution/ or acetylation method.

iii. Determination of Iodine and Saponification values of an oil sample.

iv. Determination of DO, COD and BOD of water sample.

v. Separation & identification of two compounds system.

2. Spectrophotometric (UV/VIS) Estimations 12

(i) Amino acids
(ii) Proteins
(iii) Carbohydrates
(iv) Cholesterol
(v) Ascorbic acid
(vi) Aspirin
(vii) Caffeine

or

Separation and identification of two compound system**.**

Note: Allocation of marks-Inorganic exercise 30; Organic exercise 30; Record (including test) 15; attendance 10; viva 15

SEMESTER II Paper I

Inorganic Chemistry-II

S.No.	Contents	Contact Hours/ Lecturer
1	**Metal- Ligand Bonding:** Limitations of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexesπ-bonding and molecular orbital theory.	8Lectures
2	**Reaction Mechanism of Transition Metal Complexes:** Energy profile of a reaction, reactivity of metal complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and	20 Lectures

	indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions. Complimentary and non-complimentary electron transfer reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.	
3	**Electronic Spectra and Magnetic Properties of Transition Metal Complexes** Spectroscopic ground states correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dq, B and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, magnetic properties of complexes of various geometries based on CFT, spin free- spin paired equilibrium in octahedral stereochemistry, anomalous magnetic moments, magnetic exchange coupling and spin crossover.	20 Lectures

Books Recommended:

i. F.A. Cotton, G. Wilkinson, and Paul L. Gaus, Basic Inorganic Chemistry, 3rd Edition John Wiley & Son, New York.

ii. J.D. Lee, Concise Inorganic Chemistry, 5th Edition, Wiley& Sons.

SEMESTER II Paper II

Organic Chemistry-II

S.No.	Contents	Contact Hours/ Lectures
1	**Aliphatic Electrophilic Substitution:** Biomolecular mechanisms- S_E2 and S_E1. The S_E1 mechanism, electrophilic substitution accompanied by double bonds shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity	8 Lectures
2	**Aromatic Electrophilic Substitution:** The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ispo attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling.	8 Lectures
3	**Free Radical Reactions:** Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Free radical rearrangements.	8 Lectures

4	**Addition to Carbon-Carbon Multiple Bonds:** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio-and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration..	Lectures
5	**Addition to Carbon-Hetero Multiple Bonds** Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Hydrolysis of esters and amides, ammonolysis of esters.	Lectures
6	**Elimination and Name Reactions:** The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination Vilsmeier reaction, Gattermann-Koch reaction, Sandmeyer reaction, Hunsdiecker reaction, Michael reaction. Sharpless asymmetric epoxidation, Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, Wittig reaction, Heck reaction, Still reaction, Sonogarishira, Negishi coupling, Grubbs Catalyst.	10 Lectures

BOOKS SUGGESTED:

i. Jerry March, Advanced Organic Chemistry Reactions, Mechanism and Structure, John Wiley.

ii. RT Morrison and RN Boyd Organic Chemistry, , Prentice Hall.

iii. CK Ingold, Structure and Mechanism in Organic Chemistry, Cornell University Press.

iv. SM Mukherji and SP Singh, Reaction Mechanism in Organic Chemistry, Macmillan.

v. D Nasipuri, Stereochemistry of Organic Compounds, New Age International

vi. PS Kalsi, Stereochemistry of Organic Compounds, New Age International.

vii. SM Mukherjee, Pericyclic Reactions, Macmillan, India.

viii. FA Carey and RJ Sundberg, Advanced Organic Chemistry, Plenum.

ix. Modern Organic Reactions, HO House, Benjamin.

x. Ernest L. Eliel, Samuel H Wilen, Stereochemistry of Organic Compounds, Wiley India

xi. Ernest L Eliel, Stereochemistry of Carbon Compounds. Tata McGraw Hill.

SEMESTER II Paper III

Physical Chemistry-II

S.No.	Contents	Contact Hours/ Lectures
1	**Surface and Polymer Chemistry:** Gibb's adsorption isotherm, Freundlich and Langmuir adsorption isotherms, determination of free energy of adsorption, BET theory for multilayer adsorption with derivation, determination of surface area using BET method, catalytic activity at surfaces, macromolecules, polymers and their general applications, classification of polymers, chain configuration of polymers, liquid crystals and their applications. Molecular mass, number and mass average molecular mass, molecular mass determination using osmometry, viscometry, diffusion and light scattering methods.	16Lectures
2	**Electrochemistry:** Determination of activity coefficient, Debye-Huckel theory of strong electrolytes with derivation, ionic atmosphere and thickness of ionic atmosphere, Debye-Huckel-Onsagar theory, theory of conduction, Onsagar equation including mathematical deduction, overvoltage and decomposition potential.	16 Lectures
3	**Quantum Chemistry:** de-Broglie concept and de-Broglie equation, physical interpretation and properties of wave functions, Linear, Laplacian, Linear-momentum and Hamiltonian operators, postulates of quantum mechanics, eigen values, eigen functions, normalization and orthogonalizaion, derivation of the Schrodinger's wave equation, concept of cartesian and spherical coordinates, general and brief discussion on the applications of Schrodinger's wave equation to some model systems *viz.* particles in a box, harmonic oscillator, rigid rotator and hydrogen atom.	16 Lectures

Books Recommended :

i. Puri Sharma and Pathania, Physical Chemistry, vishal Publication 2011.
ii. K.L. Kapoor, Physical Chemistry, Macllian
iii. Kinetics by Laidler, Pearson

SEMESTER II Paper IV

Spectroscopic Techniques-I

S.No.	Contents	Contact Hours/ Lectures
1	**Electron Spin Resonance Spectroscopy:** Basic Principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Hyperfine coupling isotopic and anisotropic hyperfine	16 Lectures

	coupling constants, spin Hamiltinian, spin densities, measurement techniques, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to inorganic and organic free radicals and to transition metal complexes (having an unpaired electron) including biological systems.	
2	**Nuclear Magnetic Resonance Spectroscopy:** Nuclear Spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing the chemical shift. Deshielding, spin-spin interaction, factors influencing coupling constant (J). Classification (ABX, AMX, ABC, A_2B_2 etc.), spin decoupling, basic idea about instruments, NMR studies of nuclei other than proton; ^{13}C, ^{19}F and ^{31}P. Advantages of FT NMR. Use of NMR in medical diagnostics. Simple problems and interpretation. NOE, simplification of complex spectra by the use of Shift reagent and field strength. Nuclear Overhauser Effect (NOE).^{13}C NMR spectroscopy: general considerations, chemical shift (aliphatic, olefinic, alkyne and aromatic hetero aromatic and carbonyl carbon). Coupling constants.	16 Lectures
3	**Mass Spectrometry:** Introduction, ion production-EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule, example of Mass fragmentation of organic compounds with respect to their structure determination. Problems based on spectroscopic techniques.	16 Lectures

BOOKS SUGGESTED:

i. Pavia, Lampman, Kriz, Spectroscopy, Books/Cole; Vyvyan
ii. PS Kalsi Spectroscopy of Organic Compounds, New Age International Publishers;
iii. Silverstein, Robert M.; Webster, Francis X.; Kiemle, Spectrometric Identification of Organic Compounds, John Wiley;
iv. ML Martin, JJ Delpeach and GJ Martin, Heyden, Practical NMR Spectroscopy,
v. Colin N. Banwell and Elaine M. Mc Cash, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill.
vi. RJ Abraham, J Fischer and P Loftus, Introduction to NMR Spectroscopy, Wiley.
vii. DH Williams, I Fleming, Spectroscopic Method in Organic Chemistry: Tata MacGraw Hill.
viii. Willard Merritt, Dean, Settle, Instrumental Method of Analysis: Seventh Edition, CBS, Publication.

Laboratory course: **08 hrs**

A. Physical Chemistry **30**

(i) Determination of the velocity constant of acid catalyzed hydrolysis of an ester.
(ii) Determination of activation energy of a reaction.
(iii) Determination of Frequency factor of a reaction by kinetic studies.
(iv) Validity of Arrhenius equation.
(v) Determination of the effect of change in temperature on rate constant of a reaction.
(vi) Determination of the effect of change in concentration of the reactants on rate constant of a reaction.
(vii) Determination of the effect of change in concentration of the catalyst on rate constant of a reaction.
(viii) Determination of the effect of change in ionic strength on the rate constant of a reaction.
(ix) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide.
(x) Flowing Clock reactions (Ref. Experiments in Physical Chemistry by Showmaker).
(xi) Study of the adsorption of an acid by charcoal.
(xii) Validity of Freundlich's Adsorption isotherm.
(xiii) Determination of Partition Coefficients.
(xiv) Determination of molecular surface energy of a liquid by Stalagmometer method.
(xv) Determination of association factor of the given liquid by drop-pipette method.

Note: The candidates shall have to do a minimum of 05 experiments.

B. Organic Chemistry 30

1. Multi-step Synthesis of Organic Compounds 18

The exercises should illustrate the use of organic reagent and may involve purification of the products by chromatographic techniques.

(i) Photochemical reaction:

Benzophenone ⟶ Benzpinnacol ⟶ Benzpinacolone

(ii) Beckmann rearrangement: Benzanilide from benzene

Benzene ⟶ Benzophenone ⟶ Benzophenoneoxime ⟶ Benzanilide.

(iii)Benzilic acid rearrangement: Benzilic acid from benzoin

Benzoin ⟶ Benzil ⟶ Benzilic acid

(iv) Synthesis of hetrocylic compounds

Skraup synthesis: Preparation of quinoline from aniline.

Fischer indol synthsis: Preparation of 2-phenyl indole from phenylhydrazine.

(v) Enzymatic synthesis

Enzymatic reduction: Reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S(+)ethyl-3-hydroxybetanoate and determine its optical purity.

Biosynthesis of ethanol from sucrose

(vi) Synthesis using microwaves

(vii) Alkylation of diethyl malonate with benzyl chloride.

(viii) Synthesis using phase transfer catalyst

(ix) Alkylation of diethyl malonate or ethylacetoacetate with an alkyl halide.

(x) Paper Chromatography/Thin Layer Chromatography 12

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose etc. By Paper chromatography, thin layer chromatography and determination of R_f values.

Note: Organic exercise 30; Physical 30; Record (including test) 15; attendance 10; viva15

SEMESTER III Paper I

Solid State Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Solid State Reactions, Crystal Defects and Non-stoichiometry:** General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions, Perfect and imperfect crystals, intrinsic and extrinsic defects- point defects, line and plane defects, vacancies- Schottky defects and Frenkel defects	16 Lectures
2	**Electronic Properties and Band theory:** Metals, insulators and semiconductors, electronic structure of solids-band theory. Band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors.	16 Lectures
3	**Organic Solids, Fullerenes, Molecular Devices:** Electrically conducting solids, organic charge transfer complexes, organic metals, new super conductors, magnetism in organic materials, fullerenes- doped, fullerenes as superconductors. Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches sensors.	16 Lectures

Books Recommended

i. G.W. Castellan, Physical Chemistry, 4th Ed. Narosa.

ii. R.G. Mortimer, Physical Chemistry, 3rd Ed. Elsevier: NOIDA, UP.

SEMESTER I Paper II

Spectroscope Techniques -2

S.No.	Contents	Contact Hours/ Lectures
1	**Mössbauer Spectroscopy:** Basic principles, spectral parameters and spectrum display**.** Application of the technique to the studies of (i) bonding and structure of Fe^{++} and Fe^{+++} compounds (ii) Sn^{+2} and Sn^{+4} compounds-nature of M-L bond, coordination number, structure and iii) detection of oxidation state and inequivalent MB atoms.	9 Lectures
2	**Ultraviolet and Visible Spectroscopy:** Various electronic transitions (185 to 800 nm), Lambert-Beer's Law, effect of solvent	9 Lectures

	on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, diens, conjugated polyenes. Fieser-Woodward rules for conjugated diens and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds.	
3	**Molecular Dyssemetry and Chiroptical Properties:** Linear and circularly polarized lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effects. The axial helo ketone rule, Octent diagrams, Helicity and Lowe's Rule. Application of ORD and CD to structural and stereochemical problems	7 Lectures
4	**Infrared Spectroscopy:** Instrumentation and simple handling. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the bond positions and intensities, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines and carbonyl compounds (ketones, aldehydes, esters ,amides, acids anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding, solvent effect on IR of gaseous, solids and polymeric materials. Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond. Strength' anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P,Q,R branches. Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. far IR region, metal-ligand vibrations, normal co-ordinate analysis. Simple applications.	15 Lectures
5	**Raman Spectroscopy:** Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual principles. Resonance Raman spectroscopy, Coherent anti-stokes Raman Spectroscopy (CARS), Simple applications.	8 Lectures

BOOKS SUGGESTED-

i. Pavia, Lampman, Kriz Spectroscopy, Books/Cole
ii. P. S. Kalsi, Spectroscopy of Organic Compounds, New Age International Publishers.
iii. Robert M. Silverstein, Francis X. Webster, and D. J. Kiemle Spectrometric Identification of Organic Compounds, John Wiley
iv. M. L. Martin, J. J. Delpeach G. J. Martin and Heyden, Practical NMR Spectroscopy.
v. Colin N. Banwell and Elaine M. Mc Cash, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill.
vi. R. J. Abraham, J. Fischer and P. Loftus, Introduction to NMR Spectroscopy, Wiley.
vii. D. H. Williams and I. Fleming, Spectroscopic Method in Organic Chemistry, Tata MacGraw Hill.

viii. H. H. Willard, Jr. L. L. Merritt, J. A. Dean and Jr F. A. Settle. CBS Publication. Instrumental Method of Analysis: Seventh Edition,

SEMESTER I Paper III

Chemistry of Biological System

S.No.	Contents	Contact Hours/ Lectures
1	**Bioinorganic Chemistry**: Structure and function of Cell Membrane. Essential and trace metals, role of metal ions in biological processes. Ion Transport through cell membrane. Na^+/ k^+ Pump. nitrogen fixation, metal complexes in transmission of energy, Haeme proteins and oxygen uptake, function of metalloproteins	16 Lectures
2	**Bioorganic Chemistry:** Introduction and historical perspective, Nomenclature and classification, extraction, purification and uses of enzymes in food drink industry and clinical therapy. Chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Proximity effects and molecular adaption. Enzyme kinetics, Michaelis-Mentien and Lineweaver-Burk plots, reversible and irreversible inhibition. Transition state theory, Fisher's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by site- directed, mutagenesis. Acid-base catalysis, covalent catalysis, strain or distortion. Example of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme, carboxypeptidase A and Nitrogenase. Coenzyme chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzymes A, thiamine pyrophosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid and vitamin B_{12}. Enzyme catalysed metabolic reactions	16 Lectures
3	**Biophysical Chemistry:** Forces involved in biopolymer interactions. Electrostatic charge and molecular expansion, hydrophobic forces, osmotic pressure, membrane equilibrium. Bioenergetics: Standard free energy change in biological reactions. Hydrolysis of ATP, synthesis of ATP from ADP. Coupling of ATP cleavage to endergonic processes Size, shape and molecular mass of biopolymer. Determination of molecular mass of biopolymers by various experimental techniques.	16 Lectures

BOOKS SUGGESTED

i. P.S. Kalsi, Bioorganic, Bioinorganic and Supramolecular Chemistry, New Age International.
ii. L. Stryer, Biochemistry 4th Ed., W. H. Freeman & Co.
iii. S. Zubay, Biochemistry Addison-Wesley.
iv. S. J. Lippard and J. M. Berg, Principles of Bioorganic Chemistry, University Science Books.
v. I. Berteni, H.B. Gray, S.J. Lippard and J.S. Valentine, Bioinorganic Chemistry, , University Science Books.
vi. Hermann Dugs and C. Penny, Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Springer-Verlag.
vii. Trevor Palmer, Understanding Enzymes, Prentice Hall.
viii. Collins J Sucking, Enzyme Chemistry: Impact and Application, Ed. Chapman and Hall.
ix. M.I. page and A. Williams, Enzyme Mechanisms Ed., Royal Society of Chemistry.
x. N.C. Price and L. Stevens, Fundamental of Enzymology, Oxford University Press.
xi. Michael D. Trevan, Immobilized Enzymes: An Introduction and Application in Biotechnology, John Wiley.
xii. Alan Fersht. Enzyme Reaction and Mechanism, W H Freeman & Co (Sd).
xiii. A.L. Lehninger, Principles of Biochemistry, Worth Publishers.
xiv. J. M. Berg, J. L. Tymoczko and L. Stryer, Biochemistry, W.H. Freeman.
xv. H. Robert Horton, Laurence A. Moran, Raymond S. Ochs, J. David Rawan and K. Gray Scrimgeour. Principles of Biochemistry, Neil Patterson Publishers/Prentice Hall
xvi. Donald Voet, Charlotte W. Pratt, Judith G. Voet, Biochemistry, John Wiley.
xvii. E.E. Conn and P.K. Stumpf, Outlines of Biochemistry, John Wiley.
xviii. L. S. W. H. Freeman, Macromolecules: Structure and Function, Prenctice Hall.
xix. Pramod Pandey, Organic Chemistry, John Wiley.

SEMESTER III Paper IV

Inter disciplinary topics in chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Green Chemistry:** Basic principles of green chemistry. Designing green reagents: green catalyst phase transfer catalysis for green synthesis choice of starting materials, organic synthesis in solid phase reagents, versatile ionic liquids as Scherrer methode.	10 Lectures
2	**Nano chemistry**: History, definition and scope of nanomaterials,	10

	chemical methods for synthesis of nanomaterials, methods of characterization, determination of particle size and surface structure by Scanning Electron microscopy, Transmission Electron microscopy, surface area analysis and Debye-Schrrer method	Lectures
3	**Data Analysis and Computer:** Types of errors, propagation of errors, accuracy and precision, least square analysis, average standard deviation. liner regression, co-variance and correlation coefficient. History of development of computers, Main frames, Mini, Micro and Super Computer systems. General awareness of computer hardware i.e CPU and other peripheral devices Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/Q devices, secondary storage. Computer languages. Operating system with DOS as an example. Introduction to WINDOWS. Data processing, principles of programming. Algorithms and flowcharts.	10 Lectures
4	**Environmental Chemistry:** Concept and scope, composition of atmosphere, terminology and nomenclature, aerosols, photo chemical smog, BOD and COD.	09 Lectures
5	**Medicinal Chemistry:** Primary knowledge of structure activity relationship, SAR, quantitative structure activity relationship (QSAR), Chemistry of antineoplastic agents and cardiovascular drugs	09 Lectures

Books Recommended:

i. Geoffrey A. Ozin, and Andre Arsentte, Neno Chemistry, RSC Publishing.

ii. A.K. Day, Environmental Chemistry New Age.

SEMESTER III Paper IV

Photo Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Basics of Photochemistry**: Absorption, excitation, photochemical laws, electronically excited states-life times, measurements of the times. Flash photolysis, Stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, Photochemical stages- primary and secondary processes. photo-physical reactions, Jablonskii diagram, photosensitization, quantum yield and its determination, reactions of high and low quantum yields with suitable examples, fluorescence,	6 Lectures

	phosphorescence and chemi luminiscence with suitable examples	
2	**Photochemistry of Organic Compounds:** Photochemistry of alkenes; cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3- and 1,4-dienes; dimerization.	6 Lectures
3	**Photochemistry of Carbonyl Compounds:** Norrish type I & II reactions (cyclic and acyclic); α,β-unsaturated ketones; β,γ-unsaturated ketones; cyclohexenones (conjugated); cyclohexadienons (cross-conjugated & conjugated); Paterno-Buchi reactions; photoreductions.	6 Lectures
4	**Photochemistry of Aromatic Compounds:** Isomerisation, skeletal isomerisations, Dewar and prismanes in isomerisations. Singlet oxygens reactions; Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffmann-Loefller-Freytag reaction.	6 Lectures

BOOKS SUGGESTED

i. F.A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Parts A & B, Plenum: U.S.
ii. W. M. Horspool, Aspects of Organic Photochemistry, Academic Press.
iii. T. H. Lowry and K. S. Richardson, Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc.
iv. J. March, Advanced Organic Chemistry, John Wiley & Sons.
v. L. Stryer, Biochemistry, W. H. Freeman & Co.
vi. P. A.Sykes, Guidebook to Mechanism in Organic Chemistry, Prentice-Hall.
vii. James H. Clark and Duncan J. Macquarrie, Handbook of Green Chemistry and Technology, Wiley-Blackwell.
viii. Paul T. Anastas and Tracy C. Williamson Green Chemistry: Frontiers in Benign Chemical syntheses and Processes, Oxford University Press.
ix. Geoffrey Alan Ozin, A. C. Arsenault and L. Cademartiri, Nanochemistry: A Chemical Approach to Nanomaterials, Royal Society of Chemistry.

Laboratory Course **08 hrs**

A. Physical Chemistry Practical exercises **30**

(i) Determination of the order of reaction by isolation method
(ii) Determination of the order of reaction by half life period method
(iii) Determination of the order of the reaction by Integration method.
(iv) Determination of the entropy of activation of a reaction.
(v) Determination of free energy change of a reaction.
(vi) Determination of the equilibrium constant of a reaction.
(vii) Determination of pH by electrical conductivity method.
(viii) Hydrolysis of the salts by electrical conductivity method
(ix) Hydrolysis of the salts by EMF.
(x) Determination of the dissociation constant of a weak acid by conductivity method.
(xi) Determination of the equivalent conductivity of a strong electrolyte conductometrically.

(xii) Determination of the equivalent conductivity at infinite dilution of weak electrolyte conductometrically.
(xiii) Validity of Ostwald's dilution law.
(xiv) Determination of the degree of dissociation/ association conduct metrically.
(xv) Determination of solubility and solubility product of sparingly soluble salts (e.g., $PbSO_4$, $BaSO_4$) conductometrically.

Note: The candidates shall have to do a minimum of 05 experiments

B. Inorganic Chemistry **30**

1. Quantitative analysis of binary mixture of metal ions involving volumetric (by complexometric titration using masking and demasking agents) and gravimetric analysis. 20
2. Chromatography: separation of cations and anions by paper/TLC/Ion Exchange chromatography 10

Note: Inorganic exercise 30; Physical 30; Record(including test) 15; attendance 10;viva 15

SEMESTER IV Paper I
(Elective Paper Inorganic chemistry)

General and Organometallic Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Inorganic Free Radicals:** A Comprehensive study of production, stability and reactions of free radicals: :NH, NH_2, N_2H_3 and PH.	5 Lectures
2	**Silicates and Aluminosilicates:** Silicates: Classification, properties, structure and applications of naturally occurring silicates. Aluminosilicates: chemistry of feldspars, ultramarine, zeolites, classification, structure and applications of zeolites. Clays: montmorilonite clay, synthesis of pillared clays, characterization and applications of clays and pillared clays as catalysts.	5 Lectures
3	**Organic Derivatives of Metals and Alkyls, Aryls and Acyls of Metals:** Metal beta-diketonates and thio-betadiketonates: general chemistry, structural aspects and applications. Metal alkoxides: general methods of preparation, reactivity, structure and applications Alkyls, aryls and acyls of transition metals, nature of metal carbon bond, routes of synthesis, stability, decomposition pathways, stabilization, Alkyls, aryls and acyls of s-block and p-block elements, synthesis, stability, reactivity. Comparison between transition and non-transition element derivates. Organocopper in	10 Lectures

	organic synthesis.	
4	**Compounds of Metal-Carbon Multiple Bonds and Metal Compounds with Bonds to Hydrogen:** Survey of organometallic compounds according to ligands. Synthesis, properties, nature of bonding and structural features of π-bonded organo-metallic compounds (π-complexes) with unsaturated organic molecules: alkenes, alkynes, chelating olefinic ligands, allyl, dienes-butadiene, cyclobutadiene, cyclopentadiene, fulvalene, heterocyclic pentadiene and cyclopentadienone, dienyl-cyclpentadienyl, acyclicpentadienyl, cyclohexadienyl and heptadienyl, arene and trienyl complexes. Important reactions relating to nucleophilic and electrophilic attack on ligands, role in organic synthesis. Transition metal compounds with bonds to hydrogen.	10 Lectures
5	**Homogeneous Catalysis and types of reactions**: Stoichiometric reactions for catalysis, oxidative-addition reaction, migratory inseration reaction, reductive elimination reaction, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydroformylation of olefins (oxo-reaction), Wacker's process. Activation of C-H bond, activation of small molecules by coordination	10 Lectures
6	**Fluxional Organometallic Compounds** Fluxionality and dynamic equilibria in compounds such as $\acute{\eta}^3$- allyl and dienyl complexes, their characterization.	8 Lectures

Books Recommended

i. J.P. Collman, L.S. Hegsdus, J.P. Norton and R.G. Finke, Principle and Application of Organotransition Metal Chemistry, University Science Books.

ii. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, John Wiley.

iii. A.J. Person, Metallo-organic Chemistry, Wiley.

iv. R.C. Mehrotra and A. singh, Organometallic Chemistry, New Age International.

v. J.E. Huheey, E.A. Keiter, R.L. Keiter,Inorganic Chemistry: Principle of structure and Reactivity, Pearson Education.

vi. N.L.H. Green, Organometallic Compounds, Chapman & Hall, U.K.

vii. G.E. Coates, M.L.H. Green., P. Pwell,Principles of Organometallic Chemistry, Chapman & Hall, U.K.

SEMESTER IV Paper II
(Elective Paper Inorganic chemistry)

Inorganic polymer and supramolecular Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Basics :** Importance of polymers, basic concepts: monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers, polymerization: condensation, addition, radical chain-ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions Kinetics of polymerization. Stererochemistry and mechanism of polymerization. Polymerization in homogeneous and heterogeneous systems. Comparison with organic polymers.	8 Lectures
2	**Polymer Characterization:** Polydispersion, average molecular weight concept: number average, weight average and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight: end-group, viscosity, light scattering, osmotic and ultacentrifugation methods. Analysis and testing of polymers, chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing- tensile strength. Fatigue impact. Tear resistance. Hardness and abrasion resistance.	8 Lectures
3	**Structure and Properties:** Morphology and order in crystalline polymers-configurations of polymer chains: Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point(T_M); melting points of homogeneous series, effect of chain, flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature(Tg), relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.	8 Lectures
4	**Polymer Processing :** Plastics, elastomers and fibres. Compounding. Processing techniques: calendering, die casting, rotational casting, film casting, injection moulding, extrusion moudling, thermoforming, foaming, reinforcing and fibre spinning.	8 Lectures
5	**Boron Based Polymers, Silicon Based Polymers, Phosphorous Based Polymers and Coordination Polymers:** Borazine, substituted borazines, boron nitride. Boron-oxygen-silicon and boron-oxygen-phosphorus polymers. Ployhedral borane anions. Silica, feldspars and ultramarines, silicones, silicone fluids, silicone rubbers, silicone greases, silicone resins and metallosiloxanes. Silicon-nitrogen polymers and silazenes. Metaphosphates, polyphosphates, cross-linked phosphates. Phosphonitrilic halides and related polymers. Phosphorous-sulphur polymers.	8 Lectures

	Factors affecting formation of coordination polymers. Types of coordination polymers. Metal halides. Metal pseudohalides, metal alkoxides, metal carboxylates and metal chelates	
6	**Supramolecular Chemistry: Concepts and Language** Molecular recognition: molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co-receptor molecules and multiple recognition. Strong, weak and very weak H-bonds, utilization of H-bonds to create supramolecular structures. Use of H-bond in crystal engineering and molecular recognition. Chelate and macrocyclic effects. Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules. Supramolecular reactivity and catalysis. Transport processes and carrier design. Supramolecular devices, supramolecular photochemistry, supramolecular electronic ionic and switching devices. Some examples of self-assembly in supramolecular chemistry.	8 Lectures

BOOKS SUGGESTED-

i. F.W. Bilimever Jr., Text Book of Polymer Science, Wiley.

ii. N.V. Vishwanathan and J. Sreedhar, Polymer Science, V.R. Gowarker, Willey-Eastern.
iii. K. Takemoto Y. lnaki and R.M. Ottanbrite, Functional Monomers and Polymers.
iv. H.R. Alcock and F.W. Lambe, Contemporary Polymer Chemistry, Prentice Hall.
v. J.M.G. Cowie, Physics and Chemistry of Polymers, Blakie Academic and Professional.
vi. N.H. Ray, Inorganic Polymers, Academic Press, N. York.
vii. J.M. Lehn, Supramolecular Chemistry, VCH.

SEMESTER IV Paper III
(Elective Paper Inorganic chemistry)
Photo Inorganic Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Basics of Photochemistry:** Absorption, excitation, photochemical laws, electronically excited states-life times, measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages- primary and secondary processes.	8 Lectures
2	**Photochemical Reactions:** Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry. Singlet molecular oxygen reactions. Photochemical formation of smog. Photo-degradation of polymers. Photochemistry of vision.	8Lectures

3	**Properties of Excited States and Excited States of Metal Complexes:** Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics-calculation of rates of radiative processes. Biomolecular deactivation-quenching. Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes. Charge-transfer spectra, charge transfer excitations, methods for obtaining charge-transfer spectra.	8 Lectures
4	**Ligand Field Photochemistry:** Photosubstitution, photo-oxidation and photo-reduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.	8 Lectures
5	**Redox Reactions by Excited Metal Complexes:** Energy transfer under conditions of weak interaction and strong interaction-exciplex formation, conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-phenenthroline complexes), illustration of reducing and oxidizing character of Ru^{2+}bipyridyl complex (comparison with $[Fe(bipy)_3]$); role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purpose, transformation of low energy reactants into high energy products, chemical energy into light.	8 Lectures
6	**Metal Complex Sensitizers and Determination of Reaction Mechanism :** Metal complex sensitizer, electron relay, metal colloid system, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction. Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effects of light intensity on the rate of photochemical reactions. Types of photochemical reactions; photo-dissociation, gas-phase photolysis.	8 Lectures

BOOKS SUGGESTED

i. A.W. Adamson and P.D. Fleischauer, Concept of Inorganic Photochemistry, Wiley.

ii. Inorganic Photochemistry, J. Chem. Educ., vol. 60, no. 10, 1983.
iii. .J. Lippard, Progress in Inorganic Chemistry, Vol. 30, ed. S Wiley.
iv. Coordination Chem. Revs., 1981, Vol. 39, 121, 131; 1975, 15, 321; 1990, 97, 313.
v. V. Balzari and Carassiti, Photochemistry of Coordination Compounds, Academic Press.
vi. G.J. Ferraudi, Elements of Inorganic Photochemistry, Wiley-Eastern.
vii. K.K. Rohtagi-Mukherji, Fundamentals of Photochemistry, Wiley-Eastern.
viii. A. Gilbert and J. Baggott, Essentials of Molecular Photochemistry, Blackwell Scientific Publication.
ix. N.J. Turro, W.A. Benjamin, Molecular Photochemistry,
x. A.Cox and T.Camp, Introductory Photochemistry, McGraw-Hill.
xi. R.P. Kundall and A. Gilbert, Photochemistry, Thomson Nelson.

xii. J.Coxon and B. Halton, Organic Photochemistry, Cambridge University Press.

SEMESTER IV Paper IV
(Elective Paper Inorganic chemistry)
Environmental Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Introduction to Environmental Chemistry:** Concept and scope of environmental chemistry. Environmental terminology and nomenclatures. Environmental segments. The natural cycles of environment (Hydrological, Oxygen, Nitrogen).	8 Lectures
2	**Atmosphere:** Regions of the atmosphere, reactions in atmospheric chemistry, Earth's radiation balance, particles, ion and radicals in the atmosphere. Chemistry of ozone layer.	8 Lectures
3	**Hydrosphere:** Complexation in natural water and waste-water. Micro-organism in aquatic chemical reactions. Eutrophication. Microbiology mediated redox reactions	8 Lectures
4	**Lithosphere:** Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.	8 Lectures
5	**Chemical Toxicology:** Toxic chemicals in the environments. Impact of toxic chemicals on enzymes. Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides and sulphur oxides.	8 Lectures
6	**Air Pollution and Water Pollution :** Particulates, aerosols, SOx, NOx, COx and hydrocarbon. Photochemical smog, air-quality standards. Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity). Dissolved oxygen: BOD, COD. Total organic carbon, nitrogen, sulfur, phosphorus and chlorine. Chemical speciation (Pb, As, Hg).	8 Lectures

Books Recommended:

i. Environmental Chemistry A global perspective; Fourth Edition, **Gary W. vanLoon** and **Stephen J. Duffy**

ii. Environmental Chemistry A.K. Day, New Age.

SEMESTER IV Paper V
(Elective Paper Organic chemistry)
Organic Synthesis

S.No.	Contents	Contact Hours/ Lectures
1	**Organometallic Reagents :** Principle, preparations, properties and applications of the following in organic synthesis: ***Group I and II metal organic compounds*** Li, Hg and Zn compounds. ***Transition metals:*** Pd, Ni, Fe, Ti, Cu, Rh and Cr compounds; **Other elements;** S, Si and B compounds	5 Lectures
2	**Oxidation:** Introduction. Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated & nonactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines and sulphides. Oxidation with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate. **Reduction:** Introduction, Different reductive process. Hydrocarbons-alkanes, alkenes, alkynes and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Epoxides Nitro, nitroso, azo and oxime groups. Hydrogenolysis.	10 Lectures
3	**Metallocenes, Nonbenzenoid Aromatics and Polycyclic Aromatic Compounds:** General considerations, synthesis and reactions of some representative compounds.	5 Lectures
4	**Disconnection Approach, One group C-C Disconnections and Two Group C-C Disconnections** An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions and amine synthesis. One group and two group C-C disconnections. Alcohols and carbonyl compounds, regioselectivity, Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis. Diels-Alder reaction, 1,3-difunctionalised compounds, β-unsaturated carbonyl compounds, control in carbonyl condensations. Micheal addition and Robinson annelation	15 Lectures
5	**Protecting Group**: Principle of protection of alcohol, amine,	5 Lectures

	carbonyl and carboxyl groups.	
6	**Ring Synthesis:** Saturated heterocycles, synthesis of 3-,4-,5- and 6-membered rings, aromatic heterocycles in organic synthesis.	8 Lectures

BOOKS SUGGESTED

i. H.O. House, W.A. Benjamin, Modern Synthetic Reaction,
ii. W. Carruthers, Some Modern Methods of Organic Synthesis. Cambridges Univ. Press.
iii. J. March, Advanced Organic Chemistry, Reactions Mechanisms and Structure. John Wiley.
iv. R.O.C. Norman an J.M. Coxon, Principles of Organic synthesis, Blackie Academic & Professional.
v. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part B, Plenum Press.
vi. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
vii. S Warren, Designing Organic Synthesis, Wiley.
viii. J. Fuhrhop and G. Penzillin, Organic Synthesis- Concept, Methods and Starting Materials Verlage VCH.
ix. W. A. Benjamin, Modern Synthetic Reactions, H.O. House.

SEMESTER IV Paper VI
(Elective Paper Organic chemistry)
Chemistry of Natural Products and Heterocyclic Compounds

S.No.	Contents	Contact Hours/ Lectures
1	**A. Chemistry of Natural Products** **Terpenoids and Carotenoids:** Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Menthol, Santonin and β-Carotene.	5 Lectures
2	**Alkaloids and Steroids:** Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, classification, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of Morphine and Reserpine . Occurrence, nomenclature, basic skeleton, Diel's Hydrocarbon and stereochemistry. Isolation, structure determination synthesis and biosynthesis of Cholesterol, Testosterone and Estrone.	10 Lectures
3	**Plant Pigments / Porphyrins:** Occurrence, extraction, classification, chemical characterization and functions of anthocyanins, flavonoids, xanthophylls and porphyrins. Chemistry and structure of cyanins, flavones, flavanol, quercetin. Biosynthesis of flavonoids: Acetate and Shikimic acid pathway. Structure and synthesis of porphyrin skeleton, haemin and	5 Lectures

	chlorophyll.	
4	**Prostaglandins/ Pyrethroids and Rotenones:** Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE_2 and $PGE_{2\alpha}$.Synthesis and reactions of Pyrethroids and Rotenones. Note: In structure elucidation, emphasis is to be laid on the use of spectral parameters, wherever possible.	5 Lectures
5	**Application of Spectroscopic Techniques in Structure Elucidation of Natural Products:** Two dimensional NMR spectroscopy-COSY, HETCOR, NOESY, DEPT, INEPT, APT and INADEQUATE techniques. Simplification of complex spectra-nuclear magnetic double resonance, shift reagents, solvent effects. Fourier transform technique, Nuclear Overhauser Effect (NOE). Elementary idea of NMR of , P and N nuclei	5 Lectures
6	**B. Heterocyclic Chemistry Nomenclature of Heterocycles / Aromatic and Non-aromatic Heterocycles** Systematic nomenclature (Hantzsch-Widman System) for monocyclic, fused and bridged heterocycles. Tautomerism in aromatic heterocycles. Strain-bond angle, torsional strains and their consequences in small ring heterocycles. **(i) Heterocyclic Synthesis/Small Ring Heterocycles** Three membered and four-membered 32eterocycles-synthesis and reactions of aziridines, oxiranes, thiranes, azetidines , oxetanes and thietanes. **(ii) Benzo-Fused Five-membered Heterocycles** Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes. **(iii) Six-Membered Heterocycles with Two or More Hetero atoms** Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts. Synthesis and reactions of benzopyrylium salts and coumarins. Synthesis and reactions of diazines, triazines, tetrazines and thiazines.	18 Lectures

Books Recommended

i. I. L. Finar, Vol. I & II, ELBS.
ii. Stereoselective Synthesis: A Practical Approach, M. Norgradi, VCH.
iii. Rodd's Chemistry of carbon Compounds, Ed. S. Coffey, Elsevir.
iv. Chemistry, Biological and Pharmalogical Properties of Medicinal Plants from the Americans, Ed. Kurt Hostettmann, M.P. Gupta and A. Marton, Harwood Academic Publishers.
v. Introduction to Flavonoids, B.A. Bhom, Harwood Academic Publishers.
vi. New Trends in Natural Product Chemistry, Attu-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers.
vii. Insecticides of Natural Origin, Suk Dev, Harwood Academic Publishers.
viii. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag.

ix. Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
x. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
xi. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.
xii. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon press.
xiii. Chemistry of Natural Products: A unified Approach, N.R. Krishnaswamy, Universities Press, Hyderabad.

SEMESTER IV Paper VII
(Elective Paper Organic chemistry)
Medicinal Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Drug Design :** Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drug, structure-activity relationship (SAR), factors affecting bioactivity. Theories of drug activity: general discussion. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: Lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematical derivations of equations excluded).	8 Lectures
2	**Pharmacokinetics & Pharmacodynamics :** Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process. Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.	8 Lectures
3	**Antineoplastic Agents:** Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotic and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melaphalan, uracil, mustards and 6- mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.	8 Lectures
4	**Cardiovascular Drugs:** Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output.	8 Lectures

	Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, verapamil, atenolol.	
5	**Local Anti-infective Drugs and Antibiotics:** Introduction and general mode of action. Synthesis of sulphonamides, furzolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, econozole, griseofulvin, chloroquin and primaquin. Cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxicillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.	8 Lectures
6	**Psychoactive Drugs-The Chemotherapy of Mind :** Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs –the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide.	8 Lectures

Books Suggested

i. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH
ii. Wilson and Gisvold's Text –Book of Organic Medicinal and Pharmaceutical Chemistry, Ed. Robert F. Dorge.
iii. An introduction to Drug Design, S.S. Pandeya and U.R. Diiock, New Age International.
iv. Burger's Medicinal Chemistry and Drug Discovery, Vol.- 1 (Chapter 9 and Ch-14), Ed. M.E. Wolf, John Wiley.
v. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
vi. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
vii. Strategies for Organic Synthesis and Design, D. Lednicer, John Wiley.

SEMESTER IV Paper VIII
(Elective Paper Physical chemistry)
Physical organic and Quantum Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Quantum Chemistry:** Plank's quantum theory, wave- particle duality, uncertainty principle, operators and commutation relations, degeneracy, applications of Schrodinger's wave equation to harmonic oscillator, rigid rotator and hydrogen atom, angular momentum including spin coupling of angular momentum and spin-orbit coupling. Ordinary angular momentum, generalized angular momentum,	16 Lectures

	eigen functions for angular momentum, eigen values of angular momentum, operator using ladder operators, addition of angular momentum spins, antisymmetry and Pauli 's exclusion principle.	
2	**Concepts in Molecular Orbital (MO) and Valence Bond (VB) Theory :** Introduction to Hückle Molecular Orbital (MO) method as means to explain modern theoretical methods, advanced techniques in PMO and FMO theory, molecular mechanics, semi empirical methods. Quantitative MO theory – Hückle Molecular Orbital (HMO) methods, qualitative MO theory-ionization potential, electron affinities, MO energy levels, orbital symmetry, orbital interaction diagrams, MO of simple organic systems. Valence Bond (VB) configuration mixing diagrams, relationship between VB configuration mixing and resonance theory, reaction profiles, potential energy diagrams, curve-crossing model nature of activation barrier in chemical reaction.	16 Lectures
3	**Kinetic Isotope Effect:** Theory of isotope effects, primary and secondary kinetic isotope effects, heavy atom Isotope effects. tunneling effect, solvent effects.	8 Lectures
4	**Supramolecular Chemistry:** General discussion and its importance. Molecular recognition: molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co-receptor molecules and multiple recognition. Strong, weak and very weak H-bonds, utilization of H-bonds to create supramolecular structures. Use of H-bond in crystal engineering and molecular recognition. Chelate and macrocyclic effects. Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules. Supramolecular reactivity and catalysis. Transport processes and carrier design. Supramolecular devices, supramolecular photochemistry, supramolecular electronic ionic and switching devices. Some examples of self-assembly in supramolecular chemistry.	8 Lectures

Books Suggested

i. Molecular Mechanics, Burkert and NL Allinger, ACS Monograph.

ii. Organic Chemists' Book of Orbitals, L. Salem and WL Jorgensen, Academic Press

iii. Mechanism and Theory in Organic Chemistry, TH Lowry and KC Rechardson, Harper and Row

iv. Introduction to Theoretical Organic Chemistry and Molecular Modelling,

v. W.B. Smith, VCH, Weinhelm

vi. Physical Organic Chemistry, N.S Isaacs, ELBS/Longman

vii. Supramolecular Chemistry, Concepts and Perspectives, J.M. Lehn. VCH

viii. The Physical Basis of Organic Chemistry, H Maskill, Oxford University Press.

ix. RS Molecular Mechanics, 3rd Ed., PW Atkins, Friedman, Oxford University Press (1997)

x. Quantum Chemistry 5th Ed., Ira N Levine Prentice-Hall Inc.: New Jersey

xi. Quantum Chemistry, J.P. Lowe & Peterson, Academic Press

xii. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill
xiii. Coulson's valence, R McWeeny, ELBS
xiv. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.
xv. Modern Quantum Chemistry, N. S. Ostlund and A Szabo, McGraw Hill
xvi. Methods of Molecular Quantum Mechanics, R McWeeny and BT Sutcliffe, Academic Press.
xvii. Density Functional Theory of Atoms and Molecules, RG Parr and W Yang, Oxford.
xviii. Exploring Chemistry with Electron Structure Methods, JB Foresman and E Frish, Goussian Inc
xix. Semi-empirical MO Theory, J Pople and DL Beveridge

SEMESTER IV Paper IX
(Elective Paper Physical chemistry)
Advanced Chemical Dynamics, Thermodynamics

S.No.	Contents	Contact Hours/ Lectures
1	**A. Advanced Chemical Dynamics :** Theories of reaction rates: Partition functions (translational, vibrational and rotational) for diatomic molecules and application to rate processes, statistical mechanics of chemical equilibrium, theory of absolute reaction rates, thermodynamical formulation of reactions rates, theories of unimolecular reactions: Lindemann's theory, Hinshelwood's treatment, RRK treatment, Slater's theory (no derivation), Rice-Ramsperger-Kassel-Marcus (RRKM) theory (no derivation), general treatment of chain reactions, branching chains, explosive reactions between hydrogen and oxygen, oxidation of hydrocarbons, polymerization reactions (molecular and free radical), oscillatory reactions, kinetic isotope effect.	12 Lectures
2	**Kinetics in Solution :** Influence of solvent reactions between ions, reactions between ions and molecules, reactions involving dipoles, influence of ionic strength, primary and secondary salt effects, homogeneous and heterogeneous catalysis, absolute rate theory of heterogeneous reactions. Enzyme Catalysis: Michaelis-Menton mechanism, single and double intermediates, general methods for working out the kinetics of complex enzymatic reactions.	6 Lectures
3	**Fast Chemical Reactions:** Study of kinetics by stopped flow techniques, relaxation methods, flash photolysis and magnetic resonance methods and temperature jump method.	6 Lectures
4	**B. Advanced Thermodynamics** **Statistical Thermodynamics:** Thermodynamic probability and entropy, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics Partition function: Translational, rotational, vibrational and electronic partition functions for diatomic molecules,	12 Lectures

	calculations of thermodynamic parameters and	
5	**Chemical equilibrium:** Free energy and entropy of mixing, partial molar quantities, Gibbs-Duhem equation, equilibrium constant, temperature-dependence of equilibrium constant, chemical potential and its use in heterogeneous equilibrium, fugacity, its significance and determination, ideal solutions and their properties, Duhem-Margules equation and its applicability. Dilute solutions: Lowering of melting point and elevation of boiling point, Gibb's-Helmholtz equation and its uses, Nernst heat theorem, third law of thermodynamics, entropy determination from the third law of thermodynamics.	12 Lectures

Books Suggested

i. Statistical Mechanics: Principles and Selected Application, TL Hill, Dover Publications Inc.: New York
ii. Chemical Kinetics, KJ Laidler, Mcgraw Hill
iii. Kinetics and Mechanism of Chemical Transformations, J Rajaraman and J. Kuriacose, McMillan
iv. Computer Simulations of Liquids, MP Allen and D. J. Tildesley, Oxford Science Publications: Oxford
v. Statistical Physics Vol.5, Part 1, 3rd Ed., LD Landau and IM Lifshitz, Pergamon Press
vi. Stochastic Processes in Physics & Chemistry 2nd Ed., NG van Kampen, Elsevier Science
vii. Reaction Kinetics, MJ Pilling and PW Seakins, Oxford Press
viii. Thermodynamics for Chemists, S. Glasstone
ix. Advanced Thermodynamics, RP Rastogi
x. Electrochemistry by S. Glasstone
xi. Electrochemical Methods: Fundamentals and Applications. 2nd Ed., Bard, AJ, Faulkner, L.R. John. Wiley & Sons: New York
xii. Principle of Electrochemistry, J Koryta, J Dvorak, L. Kavan, John Wiley & Sons: NY
xiii. Modern Electrochemistry, Vol I & II, JOM Bockris and AKN Readdy, Plenum.
xiv. Modern Electrochemistry, Vol I & II, JOM Bockris and AKN Readdy, Plenum

SEMESTER IV Paper X
(Elective Paper Physical chemistry)
Advanced Photochemistry and Nuclear Chemistry

S.No.	Contents	Contact Hours/ Lectures
1	**Photochemical Reactions:** Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.	8 Lectures

2	**Miscellaneous Photochemical Reactions:** Singlet molecular oxygen reactions, photochemical formation of smog and photodegradation of polymers.	8 Lectures
3	**Determination of Reaction Mechanism:** Classification, rate constants and life times of reactive energy states, determination of rate constants, effect of light intensity on the rate of photochemical reactions.	8 Lectures
4	**Molecular Photochemistry:** Transitions between states (Chemical, classical and quantum dynamics, vibronic states). Potential energy surfaces; transitions between potential energy surfaces, radiative transitions. A classical model of radiative transitions. The absorption and emission of light-state mixing, spin-orbit coupling and spin forbidden radiative transitions, absorption complexes, fluorescence, phosphorescence and chemiluminiscence.	8 Lectures
5	**Advanced Nuclear Chemistry:** Radioactive equilibrium, nuclear reaction, Q value cross section, types of reaction. Theory of Nuclear forces. Radioactive decay, alpha, beta, gamma, nuclear reactions; charecteristics and similarities with chemical reactions, threshold and cross section, nuclear reaction due to neutron, proton, deutron and gamma irradiation, Nuclear fission, fission cross section, chain fission and resonance capture. Fission products and fission yields, mass and charge distribution in fission and spallation reaction, nuclear reactor. Nuclear fission and stellar energy	16 Lectures

Books Suggested

i. Modem Molecular Photochemistry, NJ Turro, University Science Books
ii. Essentials of Molecular Photochemistry, A Gilbert, J Baggot, Blackwell Scientific
iii. Fundamentals of Photochemistry, K.K. Rohtagi-Mukharji, Wiley- Eastern.
iv. Molecular Photochemistry, NJ Turro, W.A. Benjamin.
v. Introductory Photochemistry, A Cox and T. Champ, McGraw-Hill.
vi. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
vii. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
viii. Modern molecular photochemistry, NJ Turro, University Science Books.
ix. Nuclear chemistry by Arnikar
x. Advanced Physical Chemistry, D. N. Bajpai, S. Chand and Co.
xi. Modern Physical Chemistry, Kundu and Jain, S. Chand and Co.

Organic Laboratory Course **08 hrs**

I- Qualitative Analysis **24**

Separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and one solid, two solids and one liquid), using TLC for checking the purity of the separated compounds, chemical analysis, IR, PMR and Mass Spectral data (sets of spectra may be provided to Students for characterization of components).

II- Extraction of Organic Compounds from Natural Sources (Minimum of any two of the following exercises are compulsory)
18

I) Isolation of caffeine from tea leaves.
II) Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).
III) Isolation of lactose from milk (purity of sugar should be checked by TLC, PC and Rf value reported).
IV) Isolation of nicotine dipicrate from tobacco.
V) Isolation of cinconine from cinchona bark.
VI) Isolation of piperine from black pepper.
VII) Isolation of lycopene from tomatoes.
VIII) Isolation of β-carotene from carrots.
IX) Isolation of oleic acid from olive oil (involving the preparation complex with urea and separation of linoleic acid).
X) Isolation of eugenol from cloves.
XI) Isolation of limonene from citrus fruits.

III- Spectroscopy **18**

Identification of organic compounds by the analysis of the spectral data (UV, IR, PMR, CMR & MS)

Note: Record (including test) 15; attendance 10; viva 15

Books suggested

i. Introduction to Organic Laboratory Techniques (Third Edition), DL Pavia, GM Lampman & GS Kriz, Saunders College Publishing, Phildelphia, New York.
ii. Operational organic chemistry, A Laboratory Course, Second Edition, JW Lehman. Allyn &Bacon, Inc.Boston.
iii. Microscale Organic experiments KL Willianson, DC Heath & Co Le. Xington.
iv. Laboratory Manual of Organic Chemistry, RK Bansal, New age International, Delhi
v. Vogel's Text book of quantitative Analysis, (revised), J.Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS
vi. Synthesis and Characterization of inorganic Compounds, W.L. Jolly, Prentice Hall
vii. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
viii. Macroascale and Microscale Organic Experiments, K.L. Williamson and D.C. Heath.
ix. Systematic Qualitative Organic Analysis, H. Middleton and Adward Arnold.
x. Handbook of Organic Analysis, Qualitative and Quantitative, H. Clark and Adward Arnold
xi. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
xii. Practical Physical Chemistry. A.M. James and F.E. Prichard, Longman.
xiii. Findley's Practical Physical Chemistry, B.P. Levitt Longman.
xiv. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

Physical Chemistry Lab course **08 hrs**

1. Study of complex formation by the following methods and determination of stability constant wherever practicable:
   (a) Cryoscopy

(b) Electrical Methods
(c) E.M.F.

2. Determination of transport number.
3. Determination of liquid junction potential.
4. Determination of the charge on colloidal particle.
5. Determination of λ(max) of compounds and verification of Beer's law.
6. Validity of Langmuir's adsorption isotherm.
7. Determination of partial molar volume of solute.
8. Determination of the following thermodynamic parameters of a reaction
   (a) Enthalpy of activation.
   (b) Entropy of activation.
   (c) Free energy change.
   (d) Equilibrium constant.
   (e) Frequency factor
9. Conductometric determination of the equivalent conductivity at infinite dilution of a strong electrolyte.
10. Determination of the dissociation constant of a weak acid by conductivity method.
11. Conductometric determination of the equivalent conductivity at infinite dilution of a weak electrolyte.
12. Validity of Ostwald's dilution law.
13. Determination of the degree of dissociation/ association conductometrically.
14. Determination of the formula of silver ammonia complex & copper ammonia complex.
15. Kinetic Study of the primary salt effect
16. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
17. Determination of pH by EMF.
18. Hydrolysis of the salts by cryoscopic method.
19. Determination of strengths of halides in a mixture potentiometrically.
20. Determination of the valency of mercurous ions potentiometrically.
21. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
22. Verification of the law of photo-chemical equivalence.

Note: The candidates shall have to do a minimum of 10 experiments. Record (including test) 15; attendance 10; viva 15

Inorganic Chemistry Lab course **08 hrs**

1. Semimicro analysis of inorganic mixture for six radicals. 24

2. Analysis of ores, alloys and inorganic substances by qualitative and quantitative methods. 18

   Or

   Three component metal ion analysis (one volumetric and two gravimetric methods) 18

3. Preparation 18

   Synthesis of selected inorganic compounds/ complexes and their characterization by IR, electronic spectra (UV & Visible), NMR, Mossbauer, ESR and magnetic susceptibility etc. measurements. Selection can be made from the following or any other from the existed literature.

(i) cis-and trans- isomers of $[Co(en)_2Cl_2]$ Cl.
J. Chem. Soc., 1960, 4369.

(ii) Metal acetylacetonates: $[Cr(acac)_3]$; Vanadyl acetylacetonate, $[Cu(acac)_2 . H_2O$ etc.
Inorganic Synthesis, 1957, **5**, 130; **1**, 183.

(iii) Ferrocene
J. Chem. Edu., 1996, **43**, 73; 1976, 53, 730.

(iv) Cr(II) complexes: $[Cr (H_2O)_6] (NO_3)_3 . 3H_2O$; $[Cr(H_2O)_4 Cl_2] Cl.2 H_2O$; $[Cr(en)_3]Cl_3$
Inorg. Synth., 1972, 13, 184.

(v) Tin(IV) iodine, Tin(IV) choride, Tin(II) iodine.
Inorg. Synth., 1953,4,119.

(vi) Mixed valence dinuclear complexes of manganese (III, IV).

(vii) Preparation of tripheny phosphine and its transition metal complexes.

(viii) Reaction of Cr(III) with multidentate ligand, a kinetic experiment (visible spectra of Cr-EDTA complex).
J. Am. Chem Soc., 1953,75,5670.

(ix) Other new synthesis reported in literature.

(x) Bromination of $[Cr(acac)_3]$.
J. Chem. Edu., 1986,63,90.

(xi) Preparation of copper glycine complex- cis- and trans- bis glycinato copper (II).
J. Chem. Edu., 1982,59,1052.

(xii) Relative stability of Tin (IV) and Pb (IV), preparation of ammonium hexachlorostannate, $(NH_4)[SnCl_6)$ and ammonium hexachoroplumbate; $(NH_4)_2$ $[PbCl_6]$.

Note: Record (including test) 15; attendance 10; viva 15

Note: *For conducting Chemistry Practical Examination in Semester I, II and III only One external examiner shall be appointed in each Semester. External examiners shall be appointed from all the three specialization viz; Inorganic, Organic and Physical in semester I, II and III as per syllabus.*

PROJECT WORK

In the IV Semester the candidate shall have to do a Project. The topic of the project shall be allotted to him/her by the Project Supervisor. The submission of the project shall be mandatory for each candidate and he/she will have to submit the project/dissertation not later than the date of his/her practical examination.

NOTE: Any Government PG College affiliated to the Kumaun University, if wants or have started specialized course at M. Sc. IV semester level, must seek permission from the University.

Prof. Anand B. Melkani
Convener, BOS Chemistry
Head, Department of Chemistry
Kumaun University, Nainital