KUMAUN UNIVERSITY NAINITAL



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

Effective from academic year 2022-23

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	a. Biology for Chemist (for Mathematics student)	2
courses	b. Mathematics for Chemist (for Biology student)	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	4 + 4
	group	
CHEM 40(O)	Two Elective Courses in Organic Chemistry	4 + 4
	group	

CHEM 40(P)	Two Elective Courses in Physical Chemistry	4 + 4
	group	
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(I1):General and Organometallic Chemistry

CHEM 40(I₂): Inorganic polymer and supramolecular Chemistry

CHEM 40(I₃): Photo Inorganic Chemistry CHEM 40(I₄): Environmental Chemistry

Organic Chemistry; Group-2

CHEM 40(O₁): Organic Synthesis

CHEM 40(O₂): Chemistry of Natural Products and Heterocyclic Compounds

CHEM 40(O₃): Medicinal Chemistry

Physical Chemistry; **Group-3**

CHEM 40(P1): Physical organic and Quantum Chemistry

CHEM 40(P₂): Advanced Chemical Dynamics, Thermodynamics CHEM 40(P₃): 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 two days (time 6 hours each day). The external examiner will examine the students only on the second day of examination. 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 , SnCl ₂ , TeF ₅ ⁻ , BrF ₃ , ICl ₂ ⁻ , ICl ₄ -, OF ₂ , OSF ₄ , XeF ₆ , SO ₂ , NO ₂ , NO ₂ ⁺ NO ₂ ⁻ , XeF ₂ , XeO ₃ , XeOF ₄ , and IF ₇ , dπ-pπ bonds, Isovalent hybridization, Drago Rule, Bent rule, its application and energetics of hybridization, Walsh Diagram (AB ₂ , AB ₃ and AB ₄ molecule), 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: Introduction, classification of clusters. Diborane-structure and properties. Higher boranes- Introduction, classification, STYX rule, classification and structures of carboranes. Metalloboranes and metallocarboranes. Isolobal analogy. Metal carbonyl and metalhalide clusters - Introduction, classification and structures. Zintel ions, Wade's rule for cluster compounds.	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	6 Lectures
	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 and cryptands,	
	inclusion compounds, cyclodextrins, catenanes and rotaxanes.	
2	Stereochemistry: Molecular symmetry and chirality: symmetry	
	operations and symmetry elements, point group classification and	Lectures
	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	

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	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.	
3	Pericyclic Reactions: Molecular orbital symmetry, Frontier	10
	orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl	Lectures
	system. Classification of pericyclic reactions. Woodward-	
	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	6 Lectures
	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.	
5	Aromatic Nucleophilic Substitution: The $S_N Ar$, S_N^1 , benzyne and	6 Lectures
	S_N^1 mechanism. Reactivity-effect of substrate structure leaving	
	group and attacking nucleophile. The Von-Richter, Sommelet-	
	Hauser and Smiles rearrangements.	
6	Mechanism of Carbocation Rearrangement Reactions: Pinacol-	8 Lectures
	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	

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	Lectures 24 Lectures
	coefficients, ionic strength, application of phase rule to three	
2	Chemical Dynamics: Third and general order reactions, Experimental methods for kinetic studies, <i>viz</i> ; 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. Kinetics 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 ₂ O 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	16
	elements and symmetry operations, definitions of group and	Lectures
	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.	12
2	X-ray Diffraction Methods: Bragg condition, Miller indices, Laue's method, Bragg's method, Debye- Scherrer method of X-ray	Lectures
	structural analysis of crystals. Description of the procedure for an	Lectures
	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.	
3	Chromatographic methods: Principle and classification of	15
	chromatography, Theories, Plate Theory, concept about HEPT,	Lectures
	Van-Deemter equation (no derivation) and Rate Theory.	
	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), Applications.	
4	Radio Analytical Methods: Basic principles and types of	5 Lectures
	measuring instrument, isotope dilution techniques- principle of	
<u> </u>	operations and uses. Applications.	

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(A)

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

S.No.	Contents	Contact
		Hours/
		Lectures
1	Cell as Unit of Lite: The cell theory; prokaryotic and eukaryotic	12
	and eukaryotic cells; cell size and shape; Eukaryotic cell components	Lectures
2	Cell Organelles: Mitochondria: Structure, marker enzymes,	12
	composition; function. Chloroplast: Structure, marker enzymes,	Lectures
	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	
3	Cell Membrane and Cell Wall: The functions of membranes;	12
	Models of membrane structure; faces of the membrane, selective	Lectures
	permeability of permeability of the membranes; cell wall	
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(B)

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

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

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

12 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. $[Ni(dmg)_2]$

7. Prussian Blue, Tumbull's Blue

2. $[Cu(NH_3)_4]SO_4.H_2O$

8. $Co[NH_3)_6][Co(NO_2)_6]$

3.	$Cis-K[Cr(C_2O_4)_2(H_2O)_2]$	9.	Cis-[Co(trien)(NO ₂) ₂]Cl.H ₂ O
4.	$Na[Cr(NH_3)_2(SCN)_4]$	10.	Hg [Co(SCN) ₄]
5.	$[Mn(acac)_3$	11.	$[Co(py)_2Cl_2]$
6.	$K_3[Fe(C_2O_4)_3]$	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.

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(v) Ascorbic acid(ii) Proteins(vi) Aspirin(iii) Carbohydrates(vii) Caffeine
- (iv) Cholesterol

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, Sigma bonding in octahedral complexes: Classification of metal valence orbitals into sigma symmetry, formation of ligand group orbitals (LGOs) of sigma symmetry, Formation of molecular orbitals of sigma symmetry, construction of molecular orbital energy level diagram involving only sigma bond contribution from ligands, pi bonding in octahedral complexes: Classification of metal valence orbital into pi symmetry, Formation of LGOs of pi symmetry. Formation of pi MOs and construction of molecular orbital energy level diagram involving sigma and pi contribution from pi donor ligands, Sigma and pi bonding in tetrahedral complexes and square	8Lectures
	planar complexes.	

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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 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 noncomplimentary electron transfer reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.	20 Lectures
3	Electronic Spectra and Magnetic Properties of Transition Metal Complexes: Introduction, types of transition, factors affecting band width and intensity, spectroscopic ground state terms (Russell Saunders coupling/ L-S coupling/Spin orbit coupling), determination of spectroscopic terms (p^2 and d^2 configurations), atomic terms. Microstates- calculation and representation, Mullikan terms (molecular term), splitting of atomic terms in octahedral and tetrahedral field. Correlation diagram (d^1 , d^2 configuration), Orgel diagram, (d^1 - d^9 octahedral and tetrahedral complexes), selection rules (spin and Laporte) and their relaxation. Discussion of the electronic spectrum of d^1 - d^9 octahedral and tetrahedral complexes. Inter-electronic repulsion parameters-Racah parameters (A, B, C), Nephelauxetic effect. Ground state terms symbol of transition metal complexes. Tanabe Sugano diagram (d^1 - d^9 octahedral complexes). Application of Tanabe-Sugano diagram- Calculation of B, Δ_0 , β . Charge transfer spectra- Introduction, types, factors affecting. Spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information.	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	Alinhatia Flastranhilia Substitution: Piamalagular machanisma	Q I octures
1	Aliphatic Electrophilic Substitution: Biomolecular mechanisms	8 Lectures
	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	
2	Aromatic Electrophilic Substitution: The arenium ion	8 Lectures
	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.	
3	Free Radical Reactions: Types of free radical reactions, free	8 Lectures
	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.	
4	Addition to Carbon-Carbon Multiple Bonds: Mechanistic and	Lectures
4	stereochemical aspects of addition reactions involving	Lectures
	1	
	chemoselectivity, orientation and reactivity. Addition to	
	cyclopropane ring. Hydrogenation of double and triple bonds,	
	hydrogenation of aromatic rings. Hydroboration	-
5	Addition to Carbon-Hetero Multiple Bonds Mechanism of metal	Lectures
	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.	
6	Elimination and Name Reactions: The E2, E1 and E1cB	10
	mechanisms and their spectrum. Orientation of the double bond.	Lectures
	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.	
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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,	16Lecture
	Freundlich and Langmuir adsorption isotherms, determination of	S
	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.	
2	Electrochemistry: Determination of activity coefficient, Debye-	16
	Huckel theory of strong electrolytes with derivation, ionic	Lectures
	atmosphere and thickness of ionic atmosphere, Debye-Huckel-	
	Onsagar theory, theory of conduction, Onsagar equation including	
	mathematical deduction, overvoltage and decomposition potential.	
3	Quantum Chemistry: de-Broglie concept and de-Broglie	16
	equation, physical interpretation and properties of wave functions,	Lectures
	Linear, Laplacian, Linear-momentum and Hamiltonian operators,	
	postulates of quantum mechanics, eigen values, eigen functions,	
	normalization and orthogonalization, 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 <i>viz.</i> particles	
	in a box, harmonic oscillator, rigid rotator and hydrogen atom.	

Books Recommended:

- i. Puri Sharma and Pathania, Physical Chemistry, vishal Publication 2011.
- ii. K.L. Kapoor, Physical Chemistry, MacIlian
- 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 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.	16 Lectures
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 ₂ B 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:

12 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 → Benzpinacol → Benzpinacolone

(ii) Beckmann rearrangement: Benzanilide from benzene

Benzene → Benzophenone → Benzophenoneoxime → Benzanilide.

(iii)Benzilic acid rearrangement: Benzilic acid from benzoin

Benzoin ____ 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:	16
	General principles, experimental procedures, co-precipitation as a	Lectures
	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	
2	Electronic Properties and Band theory: Metals, insulators and	16
	semiconductors, electronic structure of solids-band theory. Band	Lectures
	structure of metals, insulators and semiconductors. Intrinsic and	
	extrinsic semiconductors, doping semiconductors, p-n junctions,	
	super conductors.	
3	Organic Solids, Fullerenes, Molecular Devices: Electrically	16
	conducting solids, organic charge transfer complexes, organic	Lectures
	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.	

Books Recommended

- i. G.W. Castellan, Physical Chemistry, 4th Ed. Narosa.
- ii. R.G. Mortimer, Physical Chemistry, 3rd Ed. Elsevier: NOIDA, UP.

SEMESTER III 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	9 Lectures
2	transitions (185 to 800 nm), Lambert-Beer's Law, effect of solvent 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.	9 Lectures
3	Molecular Dyssemetry and Chiroptical Properties: Linear and	7 Lectures
	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	
4	Infrared Spectroscopy: Instrumentation and simple handling.	15
	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.	Lectures
5	Raman Spectroscopy: Classical and quantum theories of Raman	8 Lectures
	effect. Pure rotational, vibrational and vibrational-rotational Raman	
	spectra, selection rules, mutual principles. Resonance Raman	
	spectroscopy, Coherent anti-stokes Raman Spectroscopy (CARS),	
	Simple applications.	

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 III Paper III

Chemistry of Biological System

S.No.	Contents	Contact
		Hours/
		Lectures
1	Bioinorganic Chemistry: Structure and function of Cell	16
	Membrane. Essential and trace metals, role of metal ions in	Lectures
	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	
2	Bioorganic Chemistry: Introduction and historical perspective,	16
	Nomenclature and classification, extraction, purification and uses	Lectures
	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	
2	catalysed metabolic reactions	1.0
3	Biophysical Chemistry: Forces involved in biopolymer	16
	interactions. Electrostatic charge and molecular expansion,	Lectures
	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.	

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	10
	green reagents: green catalyst phase transfer catalysis for green	Lectures
	synthesis choice of starting materials, organic synthesis in solid	
	phase reagents, versatile ionic liquids as Scherrer methode.	
2	Nano chemistry: History, definition and scope of nanomaterials,	10
	chemical methods for synthesis of nanomaterials, methods of	Lectures
	characterization, determination of particle size and surface structure	
	by Scanning Electron microscopy, Transmission Electron	
	microscopy, surface area analysis and Debye-Schrrer method	
3	Data Analysis and Computer: Types of errors, propagation of	10
	errors, accuracy and precision, least square analysis, average	Lectures
	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.	
4	Environmental Chemistry: Concept and scope, composition of	09
	atmosphere, terminology and nomenclature, aerosols, photo	Lectures
	chemical smog, BOD and COD.	
5	Medicinal Chemistry: Primary knowledge of structure activity	09
	relationship, SAR, quantitative structure activity relationship	Lectures
	(QSAR), Chemistry of antineoplastic agents and cardiovascular	
	drugs	

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

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

12 hrs

30

A. Physical Chemistry Practical exercises

- (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., PbSO₄, BaSO₄) conductometrically.

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

B. Inorganic Chemistry

30

- Quantitative analysis of binary mixture of metal ions involving volumetric (by complexometric titration using masking and demasking agents) and gravimetric analysis.
- 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: Introduction, difference between ions and free radicals, inorganic and organic free radicals, types of free radical reactions, isolation of free radicals, steps involved in free radical chain reaction, kinetics of chain reaction. A Comprehensive study of production, stability and reactions of free radicals: NH, NH ₂ , N ₂ H 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	10
3	Metals: Metal beta-diketonates and thio-betadiketonates: general	Lectures
	chemistry, structural aspects and applications. Metal alkoxides:	Lectures
	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	
	organic synthesis.	
4	Compounds of Metal-Carbon Multiple Bonds and Metal	10
	Compounds with Bonds to Hydrogen: Survey of organometallic	Lectures
	compounds according to ligands. Synthesis, properties, nature of	Zectares
	bonding and structural features of π -bonded organo-metallic	
	compounds (π -complexes) with unsaturated organic molecules:	
	alkenes, Schrock and Fischer carbine, alkynes, chelating olefinic	
	ligands, allyl, dienes-butadiene, cyclobutadiene, cyclopentadiene,	
	fulvalene, heterocyclic pentadiene and cyclopentadienone, dienyl-	
	cyclpentadienyl (Metallocenes, types of metallocenes, molecular	
	orbital energy level diagram; MOED), acyclicpentadienyl,	
	cyclohexadienyl and heptadienyl, arene (MOED) and trienyl	
	complexes. Important reactions relating to nucleophilic and	
	electrophilic attack on ligands, role in organic synthesis.	
	Transition metal compounds with bonds to hydrogen.	
5	Homogeneous Catalysis and types of reactions: Difference	10
	between homogeneous and heterogeneous catalysis, oxidative-	Lectures
	addition, migratory insertion, reductive elimination, homogeneous	
	catalytic hydrogenation- Activation of hydrogen molecule-	
	oxidative addition (dihydride catalytic hydrogenation, Mechanism	
	of Wilkinson's and Schrock-Osborn catalysts), heterolytic	
	(monohydride catalytic hydrogenation, ruthenium (II) catalyst),	
	homolytic (Iguchi catalyst), Zeigler-Natta polymerization of olefins	
	by metallocenes, catalytic reactions involving carbon monoxide	
	such as hydroformylation or hydrocarboxylation of olefins (oxo-	
	reaction), Wacker's process. Activation of C-H bond, activation of	
	small molecules by coordination	0.1
6	Fluxional Organometallic Compounds: Introduction,	8 Lectures
	structural rigidity and non-rigidity, types of fluxional behavior,	
	Fluxionality and dynamic equilibria in compounds such as $\dot{\eta}^3$ - allyl	
	and dienyl complexes, their characterization.	

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	8 Lectures
	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.	
2	Polymer Characterization: Polydispersion, average molecular	8 Lectures
	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.	
3	Structure and Properties: Morphology and order in crystalline	8 Lectures
	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.	
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	8 Lectures
	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. 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	8Lectures
	with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.	
3	Properties of Excited States and Excited States of Metal	8 Lectures
	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.	
4	Ligand Field Photochemistry: Photosubstitution, photo-oxidation	8 Lectures
	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.	
5	Redox Reactions by Excited Metal Complexes: Energy transfer	8 Lectures
	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.	
6	Metal Complex Sensitizers and Determination of Reaction	8 Lectures
	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.

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	8 Lectures
	environmental chemistry. Environmental terminology and	
	nomenclatures. Environmental segments. The natural cycles of	
	environment (Hydrological, Oxygen, Nitrogen).	
2	Atmosphere: Regions of the atmosphere, reactions in atmospheric	8 Lectures
	chemistry, Earth's radiation balance, particles, ion and radicals in	
	the atmosphere. Chemistry of ozone layer.	
3	Hydrosphere: Complexation in natural water and waste-water.	8 Lectures
	Micro-organism in aquatic chemical reactions. Eutrophication.	
	Microbiology mediated redox reactions	
4	Lithosphere: Inorganic and organic components in soil, acid-base	8 Lectures
	and ion-exchange reactions in soil, micro and macro nutrients,	
	nitrogen pathways and NPK in soil.	
5	Chemical Toxicology: Toxic chemicals in the environments.	8 Lectures
	Impact of toxic chemicals on enzymes. Biochemical effects of	
	arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides	
	and sulphur oxides.	

6	Air Pollution and Water Pollution: Particulates, aerosols, SOx,	8 Lectures
	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).	

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	5 Lectures
	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	
2	Oxidation: Introduction. Different oxidative processes.	10
	Hydrocarbons-alkenes, aromatic rings, saturated C-H groups	Lectures
	(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.	
3	Metallocenes, Nonbenzenoid Aromatics and Polycyclic	5 Lectures
	Aromatic Compounds: General considerations, synthesis and	
	reactions of some representative compounds.	

4	Disconnection Approach, One group C-C Disconnections and	15
	Two Group C-C Disconnections An introduction to synthons	Lectures
	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	
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-	8 Lectures
	membered rings, aromatic heterocycles in organic synthesis.	

BOOKS SUGGESTED

- i. H.O. House, W.A. Benjamin, Modern Synthetic Reaction,
- ii. W. Carruthers, Some Modern Methods of Organic Synthesis. Cambridges Univ. Press.
- 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	5 Lectures
1	Terpenoids and Carotenoids: Classification, nomenclature,	3 Lectures
	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.	
2	Alkaloids and Steroids: Definition, nomenclature and	10
	physiological action, occurrence, isolation, general methods of	Lectures
	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.	
3	Plant Pigments / Porphyrins: Occurrence, extraction,	5 Lectures
	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 chlorophyll.	
4	Prostaglandins/ Pyrethroids and Rotenones: Occurrence,	5 Lectures
	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	Application of Spectroscopic Techniques in Structure	5 Lectures
	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).	
6	Elementary idea of NMR of , P and N nuclei P. Heterogyalia Chemistry, Nomenalature, of Heterogyalas, /	10
6	B. Heterocyclic Chemistry Nomenclature of Heterocycles / Aromatic and Non-aromatic Heterocycles	18 Lectures
	Systematic nomenclature (Hantzsch-Widman System) for	Lectures
	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.	
	i denzotutans and denzonnonienes.	

(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.	

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	8 Lectures
	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).	
2	Pharmacokinetics & Pharmacodynamics: Introduction to drug	8 Lectures
	absorption, disposition, elimination using pharmacokinetics,	o Lecture s
	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.	
3	Antineoplastic Agents: Introduction, cancer chemotherapy,	8 Lectures
	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.	
4	Cardiovascular Drugs: Introduction, cardiovascular diseases,	8 Lectures
	drug inhibitors of peripheral sympathetic function, central	2 200000
	intervention of cardiovascular output.	
	Direct acting arteriolar dilators.	
	Synthesis of amyl nitrate, sorbitrate, verapamil, atenolol.	
5	Local Anti-infective Drugs and Antibiotics: Introduction and	8 Lectures
	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.	
6	Psychoactive Drugs-The Chemotherapy of Mind: Introduction,	8 Lectures
	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.	

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	16
	duality, uncertainty principle, operators and commutation relations,	Lectures
	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,	
	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)	16
	Theory : Introduction to Hückle Molecular Orbital (MO) method	Lectures
	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.	
3	Kinetic Isotope Effect: Theory of isotope effects, primary and	8 Lectures
	secondary kinetic isotope effects, heavy atom Isotope effects.	
	tunneling effect, solvent effects.	
4	Supramolecular Chemistry: General discussion and its	8 Lectures
	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 Supramolecular devices, supramolecular photochemistry, supramolecular electronic ionic and switching devices. Some examples of self-assembly in supramolecular chemistry.

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 A I I Classical Description (TDI)	10
1	A. Advanced Chemical Dynamics: Theories of reaction rates:	12
	Partition functions (translational, vibrational and rotational) for	Lectures
	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.	
2	Kinetics in Solution : Influence of solvent reactions between ions,	6 Lectures
	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.	
3	Fast Chemical Reactions: Study of kinetics by stopped flow	6 Lectures
	techniques, relaxation methods, flash photolysis and magnetic	
	resonance methods and temperature jump method.	
4	B. Advanced Thermodynamics	12
	Statistical Thermodynamics: Thermodynamic probability and	Lectures
	entropy, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac	
	statistics Partition function: Translational, rotational, vibrational	
	and electronic partition functions for monoatomic and diatomic	
	molecules, calculations of thermodynamic parameters and partition	
	function.	
5	Chemical equilibrium: Free energy and entropy of mixing, partial	12
	molar quantities, Gibbs-Duhem equation, equilibrium constant,	Lectures
	temperature-dependence of equilibrium constant, chemical	
	1	
	potential and its use in heterogeneous equilibrium, fugacity, its	
	potential and its use in heterogeneous equilibrium, fugacity, its	

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	8 Lectures
	with matter, types of excitations, fate of excited molecule, quantum	
	yield, transfer of excitation energy, actinometry.	
2	Miscellaneous Photochemical Reactions:	8 Lectures
	Singlet molecular oxygen reactions, photochemical formation of	
	smog and photodegradation of polymers.	
3	Determination of Reaction Mechanism: Classification, rate	8 Lectures
	constants and life times of reactive energy states, determination of	
	rate constants, effect of light intensity on the rate of photochemical	
	reactions.	
4	Molecular Photochemistry: Transitions between states	8 Lectures
	(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.	
5	Advanced Nuclear Chemistry: Radioactive equilibrium, nuclear	16
	reaction, Q value cross section, types of reaction. Theory of Nuclear	Lectures
	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	

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

12 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, Scanning IR spectra of the compounds and their interpretation, chemical analysis (derivatization).

Extraction of Organic Compounds from Natural Sources (Minimum of any two of the following exercises are compulsory, recording of their IR spectra and interpretation) 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.

II- 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

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

12 hrs

- (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 $\lambda(max)$ 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

12 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

Preparation 18
 Synthesis of selected inorganic compounds/ complexes and their characterization by IR

and UV & Visible spectral data. Selection can be made from the following or any other from the existed literature.

- (i) cis-and trans- isomers of [Co(en)₂Cl₂] Cl.
 - J. Chem. Soc., 1960, 4369.
- (ii) Metal acetylacetonates: [Cr(acac)₃]; Vanadyl acetylacetonate, [Cu(acac)₂. H₂O etc. Inorganic Synthesis, 1957, **5**, 130; **1**, 183.
- (iii) Ferrocene
 - J. Chem. Edu., 1996, **43**, 73; 1976, 53, 730.
- (iv) Cr(II) complexes: [Cr (H₂O)₆] (NO₃)₃. 3H₂O; [Cr(H₂O)₄ Cl₂] Cl.2 H₂O; [Cr(en)₃]Cl₃ 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, (NH₄)[SnCl₆) and ammonium hexachoroplumbate; (NH₄)₂ [PbCl₆].

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

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

25th June, 2022