

Chemistry Syllabus

(Approved in the Board of Studies Meeting dated 9th and 10th October 2017)

Semester wise to be effective from July 2018

Note:

1. In all 72 credits are to be completed in M.Sc. out of which 18 credits shall be taken by the student in one semester.
2. In semester III and IV the student will opt one branch out of three branches i.e. Inorganic, Organic and Physical according to the availability of faculty in the department. The student will also take 18 credits in III and IV semesters out of which 9 credits i.e. two core courses will be compulsory and rest of 9 credits i.e. three courses of each three credits shall be opted out of 4 optional in each semester and in each branch.

M.S.c. I

Semester I	Course	MM	Credits
1. Inorganic Chemistry I	C001	100	3
2. Organic Chemistry I	C002	100	3
3. Physical Chemistry I (Revised)	C003	100	3
4. Group Theory & Spectroscopy	C004	100	3
5. Laboratory Course IA	C005	100	3
6. Laboratory Course IB	C006	100	3

Semester II	Course	MM	Credits
1. Inorganic Chemistry II	C007	100	3
2. Organic Chemistry II	C008	100	3
3. Physical Chemistry II	C009	100	3
4. Spectroscopy & Separation Methods	C010	100	3
5. Laboratory Course IIA	C011	100	3
6. Laboratory Course IIB	C012	100	3

M.S.c. II

Semester III	Course	MM	Credits
[A] Inorganic Chemistry			
1. Laboratory Course Inorganic IIIA	C013	100	3
2. Laboratory Course Inorganic IIIB	C014	100	3
3. Organometallic Chemistry	C015	100	3
4. Spectroscopy, X-ray & Solid State	E001	100	3
5. Bioinorganic, Bioorganic, Biophysical I	E002	100	3
6. Bioinorganic & Supramolecular Chemistry I	E003	100	3
7. Analytical Chemistry	E004	100	3
[B] Organic Chemistry			
1. Laboratory course- Organic IIIA	C016	100	3
2. Laboratory course- Organic IIIB	C017	100	3
3. Organic Synthesis & Photochem.	C018	100	3
4. Bioorganic, Bioorganic & Bio. Physical Chemistry I	E002	100	3
5. Spectroscopy & Solid State	E005	100	3

6. Organometallic reagents and Organic Synthesis	E006	100	3
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7. Medicinal Chemistry	E007	100	3
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[C] Physical Chemistry

1. Laboratory Course Physical IIIA	C019	100	3
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2. Laboratory Course Physical IIIB	C020	100	3
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3. Chemistry of Materials	C021	100	3
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4. Spectroscopy, X-ray & Solid State	E001	100	3
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5. Bioinorganic, Bioorganic and Biophysical Chemistry I	E002	100	3
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6. Analytical Chemistry	E004	100	3
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7. Liquid State	E008	100	3
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M.Sc. II

Semester IV

	Course	MM	Credits
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[A] Inorganic Chemistry

1. Laboratory Course Inorganic IVA	C022	100	3
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2. Laboratory Course Inorganic IVA	C023	100	3
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3. Inorganic Polymers	C024	100	3
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4. Spectroscopy	E009	100	3
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5. Bioinorganic, Bioorganic and Biophysical Chemistry II	E010	100	3
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6. Photoinorganic Chemistry	E011	100	3
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7. Environmental Chemistry	E012	100	3
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[B] Organic Chemistry

1. Laboratory Course Organic IVA	C025	100	3
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2. Laboratory Course Organic IVB	C026	100	3
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3. Natural Products	C027	100	3
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4. Spectroscopy	E009	100	3
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5. Bioinorganic, Bioorganic and Biophysical Chemistry II	E010	100	3
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6. Environmental Chemistry	E012	100	3
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7. Heterocyclic Chemistry	E013	100	3
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[C] Physical Chemistry

1. Laboratory Course Physical IVA	C028	100	3
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2. Laboratory Course Physical IVB	C029	100	3
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3. Advanced Quantum Chemistry	C030	100	3
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4. Spectroscopy	E009	100	3
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5. Bioinorganic, Bioorganic and Biophysical Chemistry II	E010	100	3
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6. Environmental Chemistry	E012	100	3
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7. Polymers	E014	100	3
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S.No.	Paper	Category	Paper Code	L	T	P	C
1	Inorganic Chemistry - I	Core	SOS/C001	3	0	0	3
2	Organic Chemistry - I	Core	SOS/C002	3	0	0	3
3	Physical Chemistry - I	Core	SOS/C003	3	0	0	3
4	Group Theory & Spectroscopy	Core	SOS/C004	3	0	0	3
5	Laboratory Course-IA	Core	SOS/C005	0	0	9	3
6	Laboratory Course-IB	Core	SOS/C006	0	0	9	3
7	Inorganic Chemistry - II	Core	SOS/C007	3	0	0	3
8	Organic Chemistry - II	Core	SOS/C008	3	0	0	3
9	Physical Chemistry II	Core	SOS/C009	3	0	0	3
10	Spectroscopy and Separation Methods	Core	SOS/C010	3	0	0	3
11	Laboratory Course-IIA	Core	SOS/C011	0	0	9	3
12	Laboratory Course-IIB	Core	SOS/C012	0	0	9	3
13	Laboratory Course- Inorganic IIIA	Core	SOS/C013	0	0	9	3
14	Laboratory Course- Inorganic IIIB	Core	SOS/C014	0	0	9	3
15	Organometallic Chemistry	Core	SOS/C015	3	0	0	3
16	Spectroscopy, X-ray and Solid State	Elective	SOS/E001	3	0	0	3
17	Bioinorganic, Bioorganic Biophysical Chemistry-I	Elective	SOS/E002	3	0	0	3
18	Bioinorganic and Supramolecular Chemistry	Elective	SOS/E003	3	0	0	3
19	Analytical Chemistry	Elective	SOS/E004	3	0	0	3
20	Laboratory Course-Org IIIA	Core	SOS/C016	0	0	9	3
21	Laboratory Course-Org IIIB	Core	SOS/C017	0	0	9	3
22	Organic Synthesis and Photochemistry	Core	SOS/C018	3	0	0	3
23	Spectroscopy and Solid State	Elective	SOS/E005	3	0	0	3
24	Organometallic Reagents and Organic Synthesis	Elective	SOS/E006	3	0	0	3
25	Medicinal Chemistry	Elective	SOS/E007	3	0	0	3
26	Laboratory Course Phy.-IIIA	Core	SOS/C019	0	0	9	3
27	Laboratory Course Phy.-IIIB	Core	SOS/C020	0	0	9	3
28	Chemistry of Materials	Core	SOS/C021	3	0	0	3
29	Liquid State	Elective	SOS/E008	3	0	0	3
30	Laboratory Course-Inorg. IVA	Core	SOS/C022	0	0	9	3
31	Laboratory Course-Inorg. IVB	Core	SOS/C023	0	0	9	3
32	Inorganic Polymers	Core	SOS/C024	3	0	0	3
33	Spectroscopy	Elective	SOS/E009	3	0	0	3
34	Bioinorganic, Bioorganic, Biophysical Chemistry-II	Elective	SOS/E010	3	0	0	3
35	Photoinorganic Chemistry	Elective	SOS/E011	3	0	0	3
36	Environmental Chemistry	Elective	SOS/E012	3	0	0	3
37	Laboratory Course Org.-IVA	Core	SOS/C025	0	0	9	3
38	Laboratory Course Org.-IVB	Core	SOS/C026	0	0	9	3
39	Natural Products	Core	SOS/C027	3	0	0	3
40	Heterocyclic Chemistry	Elective	SOS/E013	3	0	0	3
41	Laboratory Course Phy.-IVA	Core	SOS/C028	0	0	9	3
42	Laboratory Course Phy.-IVB	Core	SOS/C029	0	0	9	3
43	Advanced Quantum Chemistry	Core	SOS/C030	0	0	0	3
44	Polymers	Elective	SOS/E014	3	0	0	3

Semester- I

SOS/C001	Inorganic Chemistry - I	L	T	P	C	MM
		3	0	0	3	100

Unit I

Stereochemistry and Bonding in Main Group Compounds

VSEPR model and its shortcomings. Hybridization and three-center bonds. Bent's rule and energetics of hybridization.

Walsh's diagrams for tri and tetraatomic molecules. $p\pi$ - $p\pi$ and $p\pi$ - $d\pi$ bonding.

Unit II

Metal-Ligand Equilibria in Solution

Thermodynamic and kinetic stability of complexes. Stepwise and overall formation constants and their interaction. Trends in K value. Irving-Williams series. Chelate effect and its thermodynamic origin. Factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand.

Detection of complexes in solution. Determination of binary formation constants by pH-metry and spectrophotometric method.

Unit III

Reaction Mechanism of Transition Metal Complexes

Energy profile of a reaction and reactivity of metal complexes. Inert and labile complexes. Ligand substitution reactions in octahedral complexes i.e. SN^1 , SN^2 and SN^1CB mechanism. Anation reactions without metal ligand bond cleavage. Electron transfer reactions (Redox reactions). Outer and inner sphere mechanism (OSM and ISM). Reactions of coordinated ligands.

Substitution reactions in square-planar complexes.

Unit IV

Theories of Coordination Compounds

Crystal field theory, factors affecting the magnitude of Δ_0 . Consequences of crystal field splitting. Merits and limitations of CFT. Jahn-Teller distortion and its consequences on complex formation.

Evidence of covalent character in Metal-Ligand bonding. Molecular orbital theory as applied to octahedral, tetrahedral and square planar complexes.

Books suggested

- 1 Advanced Inorganic Chemistry Vth Ed., F.A. Cotton and G. Wilkinson, John Wiley, (1988).
- 2 Advanced Inorganic Chemistry VIth Ed., F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, John Wiley, (1999).
- 3 Inorganic Chemistry, J.E. House, Academic Press, (2008)
- 4 Inorganic chemistry, A Unified Approach, IInd Ed., W. W. Porterfield, Academic Press, (1993).
- 5 Coordination Chemistry, IIIrd Ed., D. Banerjee, Asian Book Pt. Ltd., (2009)
- 6 Inorganic Chemistry, 3th Ed., G. L. Miessler and D. A. Tarr, Pearson Education, Inc. (2004)
- 7 Concise Inorganic Chemistry, J. D. Lee, 5th Ed., Chapman & Hall (1996).
- 8 Inorganic Chemistry, 3rd Ed., Shriver & Atkins, Oxford (1999).
- 9 Inorganic Chemistry, 3rd Ed., Alan G. Sharpe, Addison-Wesley (1992).
- 10 Inorganic Chemistry, 4th Ed., J. E. Huheey, Harper & Row (2000).
- 11 Chemistry of the Elements, 2nd Ed., N. N. Greenwood and A. Earnshaw, Butterworth. Heinemann (1997).

- 12 Inorganic Electronic Spectroscopy, 2nd Ed., A.B.P. Lever, Elsevier (1986).
 13 Magnetochemistry, R.L. Carlin, Springer Verlag (1986).
 14 Comprehensive Coordination Chemistry Eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon (1987).

SOS/C002	Organic Chemistry - I	L	T	P	C	MM
		3	0	0	3	100

Unit I

Nature of Bonding in Organic Molecules

Hyperconjugation, bonding in fullerenes, tautomerism.

Aromaticity in benzenoid and non benzenoid compounds, alternant and non alternant hydrocarbons. Huckel's rule, energy level of π -molecular orbitals, annulenes, antiaromaticity, homo-aromaticity, PMO approach.

Bonds weaker than covalent, crown ether complexes and cryptands, inclusion compounds, cyclodextrin, catenanes and rotaxanes.

Unit II

Stereochemistry

Conformational analysis of cycloalkane, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis, chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit III

Reaction Mechanism : Structure and Reactivity

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects.

Effect of structure on reactivity – resonance and field effects, steric effect, quantitative treatments. Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

Unit IV

Aliphatic Nucleophilic Substitution

S_N1 , S_N2 and mixed S_N1 and S_N2 mechanism. The neighbouring group mechanism, neighbouring group participation (by π - and σ bonds). Anchimeric assistance. S_N1 mechanism- Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophilic group, leaving group and reaction medium, ambident nucleophile.

Unit V

Aliphatic Electrophilic Substitution

Bimolecular mechanism- $SE2$ and SEi . The $SE1$ mechanism, electrophilic substitution accompanied by double bond shift. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Books suggested:-

- Advanced Organic Chemistry, Reaction, Mechanism and Structure, Jerry March, 6th Ed., John Wiley.
- Advanced Organic Chemistry, Carey and Sundberg, Springer Verlag, Germany.
- A Guide Book to Mechanism in Organic Chemistry, Peter Sykes.

- Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
- Organic Chemistry, Boyd and Morrison, Prentice Hall of India.
- Modern Organic Reactions, H.O. House, Benjamin.
- Principles of Organic Synthesis, Norman and Coxon, Blackwell.
- Reaction Mechanism in Organic Chemistry, Mukherji and Singh, Macmillan.
- Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
- Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

SOS/C003	Physical Chemistry - I	L	T	P	C	MM
		3	0	0	3	100

Unit I :

Quantum Chemistry: Introduction to Exact Quantum Mechanical Results

The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Unit II

Quantum Chemistry: Approximate Methods

The variation theorem, linear variation principle, perturbation theory (first order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

Unit III

Quantum Chemistry: Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

Unit IV

Quantum Chemistry : Electronic Structure of Atoms

Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the p^n configuration, term separation energies for the d^n configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.

Unit V

Thermodynamics: Classical Thermodynamics

Brief resume of concepts of laws thermodynamics, free energy, chemical potential and entropies. Partial molar properties: partial molar free energy, partial molar volume and partial molar heat content and their significance. Determination of these quantities.

Concept of fugacity and determination of fugacity.

Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient.

Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength.

Unit VI

Surface Chemistry: Adsorption

Surface tension, capillary actions, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon), catalytic activity at surfaces.

Books suggested

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R. McWeeny, ELBS.

SOS/C004	Group Theory & Spectroscopy	L	T	P	C	MM
		3	0	0	3	100

Unit I

Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroups, conjugacy relation and classes. Point symmetry group, Schonflies symbols, representations of groups by matrices (representation for the C_n , C_{nv} , C_{nh} , D_{nh} etc. group to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use in spectroscopy.

Unit II

Unifying Principles

Electromagnetic radiation, interaction of electromagnetic radiation with matter. Absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, result of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-oppenheimer approximation, rotational, and electronic energy levels.

Unit III

Atomic Electronic Spectroscopy

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

Unit IV

Microwave Spectroscopy

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, Stark effect, nuclear and electron spin interaction and effect of external field. Applications.

Unit V

Infrared Spectroscopy

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, Zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy; P,Q,R branches. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region., metal-ligand vibrations.

Books Suggested:

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
3. Chemical Applications of Group Theory, F.A. Cotton.
4. Introduction of Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
5. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
6. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, New Age International.

SOS/C005	Laboratory	L	T	P	C	MM
	Course-IA	0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 12 marks each from Inorganic, Organic and Physical sections.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

Inorganic Chemistry

Qualitative Analysis

Qualitative analysis of mixtures by semi-micro methods containing not more than six cations and anions including:

- (i). Rare-earth elements
- (ii). Anions, which have not been done in under graduate practicals.
- (iii). Insolubles.

Organic Chemistry

Qualitative Analysis

Separation, purification and identification of compounds of binary mixture (solid-solid or liquid and solid) using TLC and Paper Chromatography, Chemical tests and spectroscopic analysis.

Physical Chemistry

Chemical Kinetics

1. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.

- Determination of the velocity constant of hydrolysis of an ester.
- Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics of the reaction.
- Flowing clock reactions (Ref: Experiments in Physical Chemistry by Showmaker).
- Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).

SOS/C006	Laboratory	L	T	P	C	MM
	Course-IB	0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 12 marks each from Inorganic, Organic and Physical sections.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

Inorganic Chemistry

Chromatography

Separation of cations and anions by-

Paper Chromatography

Thin Layer Chromatography

Ion Exchange Chromatography

Organic Chemistry

Organic Synthesis

Acetylation: Acetylation

Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.

Grignard reaction: Synthesis of triphenylmethanol from benzoic acid.

Sandmeyer reaction: p-Chlorotoluene from p-toluene

Physical Chemistry

Electrochemistry

Conductometry

- Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
- Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO_4 , BaSO_4) conductometrically.
- Determination of the strength of strong and weak acids in a given mixture conductometrically.
- To study the effect of solvent on the conductance of $\text{AgNO}_3/\text{CH}_3\text{COOH}$ and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
- Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law.

Semester- II

SOS/C007	Inorganic Chemistry - II	L	T	P	C	MM
		3	0	0	3	100

Unit I

Electronic Spectra & Magnetic Properties of Transition Metal Complexes.

Types of absorption spectra. Spectral terms. Russell-Saunders states. Selection rules for electronic transitions in complexes. Width of absorption spectral bands, Terms generated in ligand fields. Orgel and Tanabe-Sugano correlation diagrams for d^1 to d^9 states. Racah parameters. Charge transfer spectra. Magnetic moments, magnetic exchange coupling and spin crossover.

Unit II

Metal- π -Complexes and organometallic Compounds.

Metal carbonyl complexes. Preparation, properties and uses. Nature of bonding in metal carbonyls and carbon monoxide analogs i.e. nitrosyls and dinitrogen complexes. Evidence for back bonding in complexes.

Nature of M-C bond Synthesis, bonding and uses of organometallic compounds, two electron ligands (olefinic and acetylenic complexes), three electron ligands (allylic complexes), four electron ligand (butadiene and cyclobutadiene complexes), five electron ligand (ferrocene complexes).

Unit III

Metal Clusters

Polyhedral boranes and boran anions. Synthesis, reactivity, bonding and topology of boranes.. Wade's rules. Carboranes, metalloboranes and metallocarboranes.

Metal carbonyls and halides as clusters. Metal carbonyl hydrides.

Unit IV

Silicates

Principles of silicates. Structure and classification of silicates. Asbestos, Zeolites and Ultramarines as silicate materials. Silicates in technology

Books suggested

1. Advanced Inorganic Chemistry Vth Ed., F.A. Cotton and G. Wilkinson, John Wiley, (1988).
2. Advanced Inorganic Chemistry VIth Ed., F.A. Cotton, G Wilkinson, C.A. Murillo and M. Bochmann, John Wiley,(1999).
3. Inorganic Chemistry, J.E.House, Academic Press, (2008)
4. Inorganic chemistry, A Unified Approach, IInd Ed., W W. Porterfield, Academic Press,(1993).
5. Coordination Chemistry ,IIIrd Ed., D Banerjea, Asian Book Pt. ltd.,(2009)
6. Inorganic Chemistry, 3th Ed., G L Miessler and D.A.Tarr, Pearson Education,Inc. (2004)
7. Concise Inorganic Chemistry, J.D. Lee, 5th Ed., Chapman & Hall (1996).
8. Inorganic Chemistry, 3rd Ed., Shriver & Atkins, Oxford (1999).
9. Inorganic Chemistry, 3rd Ed., Alan G. Sharpe, Addison-Wesley (1992).
10. Inorganic Chemistry, 4th Ed., J.E. Huheey, Harper & Row (2000).
11. Chemistry of the Elements, 2nd Ed., N.N. Greenwood and A. Earnshaw, Butterworth. Heinemann (1997).
12. Inorganic Electronic Spectroscopy, 2nd Ed., A.B.P. Lever, Elsevier (1986).
13. Magnetochemistry, R.L. Carlin, Springer Verlag (1986).
14. Comprehensive Coordination Chemistry Eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon (1987).

SOS/C008	Organic Chemistry - II	L	T	P	C	MM
		3	0	0	3	100

Unit I

Aromatic Electrophilic Substitution

Orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrate and electrophiles. Diazonium coupling, Vilsmeier Haack reaction, Gattermann-Koch reaction.

Unit II

Aromatic Nucleophilic Substitution

The S_NAr, S_N1, benzyne and S_{RN}1 mechanisms. Reactivity- effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

Unit III

Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism of an aromatic substrate, neighboring 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, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Unit IV

Addition to Carbon-Carbon Multiple Bonds

Mechanism and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

Unit V

Addition to Carbon-Hetero Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Wittig reaction.

Mechanism of condensation reactions involving enolates- Knoevenagel, Claisen, Mannich Benzoin, Perkin and Stobbe reactions.

Hydrolysis of esters and amides, ammonolysis of esters.

Unit VI

Elimination Reactions

The E₂, E₁ and E_{1c}B mechanisms and their stereochemistry. Orientation of the double bond. Reactivity- effects of substrate structures, attacking base, the leaving group and the medium.

Mechanism and orientation in pyrolytic elimination.

Unit VII

Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann.

Correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and suprafacial additions, $4n$, and $4n+2$ systems. Cycloadditions-antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, $2+2$ addition of ketenes, 1, 3 dipolar cycloadditions and cheletropic 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.

Books suggested:-

1. Advanced Organic Chemistry- Reaction, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackwell.
8. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

SOS/C009	Physical Chemistry II	L	T	P	C	MM
		3	0	0	3	100

Unit I

Chemical Dynamics

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction), homogeneous catalysis, kinetics of enzymes reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.

Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

Unit II

Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws- (using Lagrange's method of undetermined multipliers).

Partition functions- translational, rotational, vibrational and electronic partition functions.

Calculation of thermodynamic properties in terms of partition functions. Applications of partition functions.

Heat capacity behaviour of solids- chemical equilibria and chemical equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal.
Bose-Einstein statistics – distribution law and application to helium.

Non-Equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

Unit III

Electrochemistry

Electrochemistry of solutions, Debye-Huckel, Onsager treatment and its extension, ion solvent interactions. Thermodynamics of electrified interface equations. Structure of electrified interfaces. Guoy Chapman, Stern. Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot.

Semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Electrocatalysis – influence of various parameters. Hydrogen electrode. Bioelectrochemistry, threshold membrane phenomena. Polarography theory, Ilkovic equation, half wave potential and its significance. Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and prevention methods.

Books suggested:-

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Coulson's Valence, R. McWeeny, ELBS.
3. Modern Electrochemistry, Vol. I & II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
7. Quantum Chemistry, Ira N. Levine, Prentice Hall.

SOS/C010	Spectroscopy and Separation Methods	L	T	P	C	MM
		3	0	0	3	100

Unit I

Molecular Electronic Spectroscopy

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of excited states, Franck-Condon principle, Dissociation and pre-dissociation, electronic spectra of polyatomic molecules. Emission spectra, radiative and non-radiative decay, internal conversion,

Unit II

Raman Spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectroscopy, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

Unit III

Magnetic Resonance Spectroscopy

Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factor influencing chemical shift, deshielding, spin-spin interaction, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A₂B₂ etc.), spin decoupling, basic ideas about instrument, NMR studies of nuclei other than proton-¹³C, ¹⁹F and ³¹P. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

Unit IV

Chromatographic Methods

Principle, instrumentation and applications of gas liquid chromatography and HPLC. Ion exchange chromatography: cationic and anionic exchanges and their applications. Van-Deemter equation (no derivation), concept about HEPT-plate theory and rate theory. Applications.

Unit V

Radio Analytical Methods

Basic principles and types of measuring instruments, isotope dilution techniques: principle of operations and uses. Applications.

Books Suggested:

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
3. Physical Method for Chemistry, R.S. Drago, Saunders Company.
4. Introduction of Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
5. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
6. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
7. Introduction to Magnetic Resonance, A. Carrington, A.D. Maclachlan, Harper & Row.
8. High Performance Liquid Chromatography, **Heinz** Engelhardt.
9. Instrumental Methods of Chemical Analysis, Willard, Meritt, Dean & Settle (Wiley Eastern).

SOS/C011	Laboratory Course-IIA	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 12 marks each from Inorganic, Organic and Physical sections.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

Inorganic Chemistry

Quantitative Analysis

Quantitative Analysis of mixtures of two metal ions involving Volumetric (by complexometric titration using masking and demasking agents) and gravimetric analysis.

Organic Chemistry

Organic Synthesis

Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.

Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate

Aromatic electrophilic Substitutions: Synthesis of p-nitroaniline and p-bromoaniline.

The products may be characterized by Spectral Techniques where possible.

Physical Chemistry

Solutions

1. Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
2. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

SOS/C012	Laboratory Course-IIB	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 12 marks each from Inorganic, Organic and Physical sections.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

Inorganic Chemistry

Preparations

Preparation of selected inorganic compounds:

VO (acac)₂

TiO (C₉H₈NO)₂. 2H₂O

cis-K[Cr(C₂O₄)₂ (H₂O)₂]

Na[Cr(NH₃)₂(SCN)₄]

Mn (acac)₃

K₃ [Fe (C₂O₄)₃] 3H₂O

Prussian Blue, Turnbull's Blue

Co [(NH₃)₆] Cl₃

[Cu (en)₂ (H₂O)₂] I₂

Cu₂HgI₄

[Co (Py)₂Cl₂]

[Ni (NH₃)₆] Cl₂

Tris-(thiourea) copper (I) sulphate [Cu (tu)₃] SO₄.2H₂O

K₃[Cr (C₂O₄)₃]

Organic Chemistry

Quantitative Analysis

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

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

Determination of Iodine and Saponification values of an oil sample

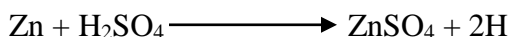
Determination of DO, COD and BOD of water sample.

Physical Chemistry

Electrochemistry

Potentiometry/pH-metry

1. Determination of strengths of halides in a mixtures potentiometrically.
2. Determination of the valency of mercurous ions potentiometrically.
3. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
4. Determination of temperature dependence of EMF of a cell.
5. Determination of the formation constant of silver-ammonia complex and stiochiometry of the complex potentiometrically.
6. Acid-base titration in a non-aqueous media using a pH meter.
7. Determination of activity and activity coefficient of electrolytes.
8. Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
9. Determination of the dissociation constant of monobasic/dibasic by Albert-Serjeant method.
10. Determination of thermodynamic constants ΔG , ΔS and ΔH for the reaction by e.m.f. method.



Semester- III

Inorganic Chemistry

SOS/C013	Laboratory Course- IIIA Inorganic	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 36 marks.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

Preparation

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

- (i). Cis and Trans isomers of $[\text{Co}(\text{en})_2\text{Cl}_2] \text{Cl}$.
J. Chem. Soc., 1960, 4369.

- (ii). Metal acetylacetonates: $\text{Cr}(\text{acac})_3$; Vanadyl acetylacetonate, $\text{Cu}(\text{acac})_2 \cdot \text{H}_2\text{O}$ etc. Inorg. Synth., 1957, 5, 130; 1, 183.
- (iii). Ferrocene
J. Chem. Edu., 1966, 43, 73; 1976, 53, 730.
- (iv). Cr(III) complexes: $[\text{Cr}(\text{H}_2\text{O})_6](\text{NO}_3)_3 \cdot 3\text{H}_2\text{O}$; $[\text{Cr}(\text{H}_2\text{O})_4 \text{Cl}_2] \text{Cl} \cdot 2\text{H}_2\text{O}$; $[\text{Cr}(\text{en})_3]\text{Cl}_3$
Inorg. Synth., 1972, 13, 184.
- (v). Tin (IV) iodide, Tin (IV) chloride, Tin (II) iodide.
Inorg. Synth., 1953, 4, 119.
- (vi). Mixed valence dinuclear complexes of manganese (III, IV).
- (vii). Preparation of triphenyl 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 $\text{Cr}(\text{acac})_3$.
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, $(\text{NH}_4)_2\text{SnCl}_6$ and ammonium hexachloroplumbate; $(\text{NH}_4)_2 \text{PbCl}_6$.

Books Suggested

1. Vogel's Text Book of Qualitative Analysis, ELBS .
2. Vogel's Text Book of Quantitative Analysis, ELBS.
3. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.

SOS/C014	Laboratory Course-IIIB	L	T	P	C	MM
	Inorganic	0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 36 marks.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

Analysis of ores, alloys and inorganic substances by various chemical methods.

Books Suggested

1. Vogel's Text Book of Qualitative Analysis, ELBS .
2. Vogel's Text Book of Quantitative Analysis, ELBS.
3. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.

SOS/C015	Organometallic Chemistry	L	T	P	C	MM
		3	0	0	3	100

I. Alkyls and Aryls of Transition Metals

Alkyls and aryls of transition metals, nature of metal carbon bond, routes of synthesis, stability and decomposition pathways and their structure. Alkyls and aryls of s-block and p-block elements. Comparison of such transition and non-transition element derivatives. Organocopper in organic synthesis.

II. Compounds of Transition metal-carbon multiple bonds

Alkylidenes, alkyldynes, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

III. Transition Metal π -Complexes

Transition Metal π -Complexes with unsaturated organic molecules. Alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes; preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

IV. Metal Compounds with bonds to Hydrogen

Transition metal compounds with bonds to hydrogen.

V. Homogeneous Catalysis

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reaction, activation of C-H bond.

VI. Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as η^2 -olefin, η^3 -allyl and dienyl complexes, their characterization.

Books Suggested:

1. Principle and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.P. Norton and R.G. Finke. University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh; New Age International.
5. Organometallic Compounds, NLH Green, Chapman & Hall, U.K.
6. Principles of Organometallic Chemistry, G.E. Coates, MLH Green, P. Powell, Chapman & Hall, U.K.

SOS/E001	Spectroscopy, X-ray and Solid State	L	T	P	C	MM
		3	0	0	3	100

I. Ultraviolet and Visible Spectroscopy

Instrumentation, source, monochromators, detectors, single and double beam instruments, applications.

II. Infrared Spectroscopy

Instrumentation, source, monochromators, optics of double beam instruments, detectors, sample preparation, applications.

III. X-Ray Diffraction

Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

IV. Electron Diffraction

Scattering intensity vs. scattering angle, Wire equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

V. Neutron Diffraction

Scattering of neutrons by solids and liquids, magnetic scattering, measuring techniques. Elucidation of structure of magnetically ordered unit cell.

VI. Solid State Chemistry

Solid State Reactions

General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

Books Suggested:

1. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
4. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
5. Solid State Chemistry and its Applications, A.R. West, Plenum.
6. Solid State Chemistry, D.K. Chakrabarty, New Age International.
7. Symmetry and Spectroscopy, K. Veera Reddy, New Age International, 1998.
8. Instrumental Methods of Analysis, Willard et al., 7th Edn., CBS Publishers.

SOS/E002	Bioinorganic, Bioorganic Biophysical Chemistry-I	L	T	P	C	MM
		3	0	0	3	100

A) Bioinorganic Chemistry

I. Metal Ions in Biological Systems, Na⁺/K⁺ Pump

Essential and trace metals. Role of metal ions in biological processes. Na⁺/K⁺ Pump.

II. Bioenergetics and ATP Cycles

DNA polymerization, glucose storage, metal complexes in transmission of energy; chlorophylls, photo system I and photo system II in cleavage of water. Model systems.

III. Transport and Storage of Dioxygen

Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

B) Bioorganic Chemistry

I. Enzymes & Mechanism of Enzyme Action

Introduction and historical perspective, chemical and biological catalysis, properties of enzymes-catalytic power, specificity and regulation. Fischer's lock and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed, mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition. Transition-state theory, acid-base catalysis, covalent catalysis, strain of distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

II. Kinds of Reactions Catalysed by Enzymes

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, β-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

C) Biophysical Chemistry

I. Biological Cell and its Constituents, Cell Membrane and Transport of Ions

Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition. Structure and functions of cell membrane, ion transport through cell membrane.

II. Bioenergetics

Standard free energy change in biological reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

Books Suggested

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Bioinorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.

4. Understanding Enzymes, Trevor Palmer, Prentice Hall.
5. Enzyme Chemistry: Impact and Applications, Ed. Colliins J Sucking, Chapman and Hall.
6. Enzymes Mechanism Ed, M.I. Page and A. Williams, Royal Society of Chemistry.
7. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.
8. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
9. Enzymatic Reaction Mechanism, C. Walsh, W.H. Freeman.
10. Enzymatic Structure and Mechanism, W.H. Freeman.
11. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
12. Biochemistry, L. Stryer, W.H. Freeman.
13. Biochemisty, J. David Rawn, Neil Patterson.
14. Biochemistry, Voet and Voet, John Wiley.
15. Outlines of Biochemistry, E.E. Conn and P.K. Stumpf, John Wiley.
16. Macromolecules: Structure and function, F. World, Prentice Hall.

SOS/E003	Bioinorganic and Supramolecular Chemistry	L	T	P	C	MM
		3	0	0	3	100

Unit I

Metal Storage Transport and Biomineralization

Ferritin, Transferrin, and siderophores

Unit II

Calcium in Biology

Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins.

Unit III

Metalloenzymes

Zinc enzymes-carboxypeptidase and carbonic anhydrase. Iron enzymes-catalase, peroxidase and cytochrome P-450. Copper enzymes-superoxide dismutase. Molybdenum oxatransferase enzymes-xanthine oxidase. Coenzymes vitamin B₁₂.

Unit IV

Metal-Nucleic Acid Interactions

Metal ions and metal complex interactions. Metal complexes-nucleic acids.

Unit V

Metals in Medicine

Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

Unit VI

Supramolecular Chemistry

Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co-receptor molecules and multiple recognition. H-bonds in

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.

Books Suggested:

1. Supramolecular Chemistry, J.M. Lehn, VCH.
2. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
3. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
4. Inorganic Biochemistry, vols I and II. Ed. G.L. Eichhorn, Elsevier.
5. Progress in inorganic Chemistry, vols 18 and 38 ed. J.J. Lippard, Wiley.

SOS/E004	Analytical Chemistry	L	T	P	C	MM
		3	0	0	3	100

Unit I

Introduction

Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations-dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.

Unit II

Errors

Determinate and indeterminate errors, minimization of determinate errors, random distribution of indeterminate errors.

Unit III

Statistical data analysis

Accuracy and precision, significant figures and computations, mean and standard deviation, distribution of random errors, reliability of results, confidence interval, comparison of results, comparison of means of two samples, paired t-test, number of replicate determinations and its use, correlation and regression, linear regression, analysis of variance, rejection of data.

Unit IV

Application of analytical chemistry in the study of water and soil pollutions, analysis of fuel, body fluids and drugs

Books Suggested:

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W.B. Saunders.
3. Analytical Chemistry-Principles, J.H. Kennedy, W.B. Saunders.

- Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
- Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W.B. Saunders.
- Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
- Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.
- Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
- Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.

Organic Chemistry

SOS/C016	Laboratory Course- Org IIIA	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 36 marks.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

Qualitative Analysis

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. Preparation of derivatives and spectral analysis.

Books Suggested

- Introduction to Organic Laboratory Techniques (Third Edition), DL Pavia, GM Lampman and GS Kriz, Saunders College Publishing, Philadelphia, New York.
- Operational Organic Chemistry, A Laboratory Course, Second Edition, JW Lehman, Allyn & Bacon, Inc. Boston.
- Microscale Organic Experiments KL Willianson, DC Health & Co. Le Xington.
- Laboratory Manual of Organic Chemistry, RK Bansal, New Age International, Delhi.

SOS/C017	Laboratory Course-Org IIIB	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 36 marks.

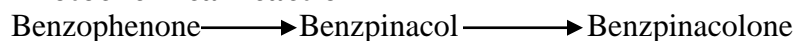
Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

Multi-step Synthesis of Organic Compounds

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

Photochemical reaction



Beckmann rearrangement: Benzanilide from benzene

Benzene \longrightarrow Benzophenone \longrightarrow Benzophenone oxime \longrightarrow Benzanilide

Benzilic acid rearrangement: Benzilic acid from benzoin

Benzoin \longrightarrow Benzil \longrightarrow Benzilic acid

Synthesis of heterocyclic compounds

Skraup synthesis: Preparation of quinoline from aniline. Fisher-Indole synthesis: Preparation of 2-phenyl indole from phenylhydrazine.

Enzymatic Synthesis

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

Biosynthesis of ethanol from sucrose

Synthesis using microwaves

Alkylation of diethyl malonate with benzyl chloride.

Synthesis using phase transfer catalyst.

Alkylation of diethyl malonate or ethylacetoacetate with an alkyl halide.

Books Suggested

1. Introduction to Organic Laboratory Techniques (Third Edition), DL Pavia, GM Lampman and GS Kriz, Saunders College Publishing, Philadelphia, New York.
2. Operational Organic Chemistry, A Laboratory Course, Second Edition, JW Lehman, Allyn & Bacon, Inc. Boston.
3. Microscale Organic Experiments KL Willianson, DC Health & Co. Le Xington.
4. Laboratory Manual of Organic Chemistry, RK Bansal, New Age International, Delhi.

SOS/C018	Organic Synthesis and Photochemistry	L	T	P	C	MM
		3	0	0	3	100

Unit I

Disconnection Approach

An introduction to synthons and synthetic equivalents disconnection approach, functional group interconversions, the importance of 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.

Unit II

Protecting Groups

Principle of protection of alcohols, amine, carbonyl and carboxyl groups

Unit III

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-difunctional compounds, α,β -unsaturated carbonyl compounds, control in carbonyl condensations. Micheal addition and Robinson annelation.

Unit IV

Determination of Reaction Mechanism

Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions, photo-dissociation, gas-phase photolysis.

Unit V

Photochemical Reactions

Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4-and 1,5-dienes.

Intramolecular reactions of carbonyl compounds-saturated cyclic and acyclic, β,γ -unsaturated and α,β -unsaturated compounds. Cyclohexadienones.

Intramolecular cycloaddition reactions-dimerisation and oxetane formation.

Isomerisation, additions and substitutions.. Photo-Fries rearrangement, Barton reaction.

Books Suggested:

1. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.
4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, Plenum Press.
6. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
7. Designing Organic Synthesis, S. Warren, Wiley.
8. Organic Synthesis-Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlag VCH.
9. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, New Age International
10. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication
11. Molecular Photochemistry, N.J. Turro, W.A. Benjamin
12. Introductory Photochemistry, A. Cox and T. Camp, McGraw Hill
13. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson
14. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press

SOS/E005	Spectroscopy and Solid State	L	T	P	C	MM
		3	0	0	3	100

Unit I

Ultraviolet

and Visible Spectroscopy

Effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds.

Unit II

Infrared Spectroscopy

General idea of the vibrational frequencies of aliphatic and aromatic hydrocarbons, amines, carbonyl compounds, acid and acid derivatives and conjugated carbonyl compounds, effect of hydrogen bonding and solvent on IR.

Unit III

Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)

Definition, deduction of absolute configuration and octant rule for ketones.

Unit IV

Solid State Chemistry

(a). Solid State Reactions

General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

(b). Organic Solids, Fullerene, Molecular devices

Electrically conducting solids, organic charge transfer complex, organic metals, magnetism in organic materials, fullerenes and doped fullerenes, organic superconductors, molecular rectifiers, transistors, artificial photosynthetic devices, molecular memory, switches and sensors.

Books Suggested

1. Physical Method for Chemistry, R.S. Drago, Saunders Company.
2. Structural Method in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Craddock, ELBS.
3. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
4. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
5. Solid State Chemistry and its Applications, A.R. West, Plenum.
6. Solid State Chemistry, D.K. Chakrabarty, New Age International.

SOS/E006	Organometallic Reagents and Organic Synthesis	L	T	P	C	MM
		3	0	0	3	100

Unit I

Principles, preparations, properties and applications of the following in organic synthesis with mechanistic details.

Group I and II metal organic compounds

Li and Hg compounds.

Transition metals

Pd, Ni and Cr compounds.

Other elements

Si and B compounds.

Unit II

Oxidation

Introduction. Different oxidative processes.

Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and inactivated).

Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids.

Amines, hydrazines, and sulphides.

Oxidations with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate.

Unit III

Reduction

Introduction. Different reductive processes.

Reduction of hydrocarbons- alkenes, alkynes and aromatic rings.

Reduction of carbonyl compounds (aldehydes, ketones, acids and their derivatives). Epoxides.

Reduction of nitro, nitroso, azo and oxime groups.

Hydrogenolysis.

Unit IV

Rearrangements

General mechanistic considerations-nature of migration, migratory aptitude, memory effects

A detailed study of the following rearrangements

Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction

Unit V

Metalloenes, Nonbenzenoid Aromatics and Polycyclic Aromatic Compounds

General considerations, synthesis and reactions of some representative compounds

Books Suggested:

1. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, 6th Edn., John Wiley.
4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, Plenum Press.
6. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
7. Designing Organic Synthesis, S. Warren, Wiley.
8. Organic Synthesis-Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlag VCH.

SOS/E007	Medicinal Chemistry	L	T	P	C	MM
		3	0	0	3	100

Unit I

Drug Design

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR) factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. 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 constant, 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).

Unit II

Pharmacokinetics

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

Unit III

Pharmacodynamics

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotic, biotransformation, significance of drug metabolism in medicinal chemistry.

Unit IV

Antineoplastic Agents

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards, and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

Unit V

Antibiotics

Cell wall biosynthesis inhibitors, β -lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxicillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

Books suggested

1. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH.
2. Wilson and Gisvold's: Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed. Robert F. Dorge.
3. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol-I, Ed. M.E. Wolff, John Wiley.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
6. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
7. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

Physical Chemistry

SOS/C019	Laboratory Course Phy.IIIA	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 36 marks.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

1. Verification of the law of photochemical equivalence.
2. Order of reaction by:
 - (a). Isolation Method.
 - (b). Half life period method
 - (c). Integration method
3. Temperature coefficient of a reaction.
4. Energy of activation of a reaction.
5. Entropy of a reaction.
6. Determination of pH by following methods:
 - (a). Electrical Conductivity.
 - (b). E.M.F.
 - (c). Polarography

SOS/C020	Laboratory Course Phy.-IIIB	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do one exercise of 36 marks.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

1. Hydrolysis of the salts by following methods:
 - (a). Cryoscopic
 - (b). Electrical Conductivity.
 - (c). E.M.F.
2. Study of complex formation by the following methods and determination of stability constant wherever practicable:
 - (a). Cryoscopic
 - (b). Electrical Methods.
 - (c). E.M.F.
3. Determination of solubility of sparingly soluble salts by the following methods:
 - (a). Electrical Conductivity.
 - (b). E.M.F.
4. Dissociation constants of polybasic acids.

SOS/C021	Chemistry of Materials	L	T	P	C	MM
		3	0	0	3	100

Unit I

Multiphase Materials

Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications

Unit II

Glasses, Ceramics, Composites and Nanomaterials

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and applications.

Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.

Unit III

Thin Films and Langmuir-Blodgett Films

Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc.

Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

Unit IV

Liquid Crystals

Mesomorphic behavior, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic-nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

Unit V

Polymeric Materials

Molecular shape, structure and configuration, crystallinity, stress-strain behavior, thermal behavior, polymer types and their applications, conducting and ferro-electric polymers.

Unit VI

Ionic Conductors

Types of ionic conductors, mechanism of ionic conductors, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

Unit VII

High T_c Materials

Defect perovskites, high T_c superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high T_c materials, applications of high T_c materials.

Books Suggested

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D. Callister, Wiley.
3. Principles of the Solid State, H.V. Keer, Wiley Eastern.
4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS.
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. Handbook of Liquid Crystals, Kelker and Hatz, Chemie Verlag.
7. Inorganic Materials:Recent Advances,Editors D.Bahadur *et al.*,Narosa
8. Ion Conducting Materials: Theory and Applications, Editor A. R. Kulkarni, Narosa.

SOS/E008	Liquid State	L	T	P	C	MM
		3	0	0	3	100

Unit I

General Properties of Liquids

(a) Liquids as dense gases, liquids as disordered solids, some thermodynamics relations, internal pressure and its significance in liquids. Equations of state, critical constants. Different types of intermolecular forces in liquids, different potential functions for liquids. Additivity of pair potential approximation.

(b) A classical partition function for liquid for liquids, correspondence principle, configuration integral, configuration properties.

Unit II

Theory of Liquids

Theory of liquids, partition function method or model approach, single cell models, communal energy and entropy, LTD model, significant structure model.

Unit III

Distribution Function and Related Equations

Radial distribution function method, equation of state in terms of RDF, Molecular distribution functions, pair distribution function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion.

Unit IV

Methods for Structure Determination and Computational Techniques

Spectroscopic techniques for liquid dynamic structure studies, Neutron and X-ray scattering spectroscopy.

Computation Techniques- Monte Carlo and molecular dynamics methods.

Unit V

Supercooled and Ionic Liquids.

Supercooled and ionic liquids, theories of transport properties; non Arrhenius behavior of transport properties, Cohen-Turnbull free volume model, configurational entropy model, Macedo-Litovitz hybrid model, glass transition in supercooled liquids.

Books Suggested

1. An Introduction to Liquid State, P.A. Egeistaff, Academic Press.
2. The Dynamic Liquid State, A.F.M. Barton, Longman.
3. Introduction to Statistical Thermodynamics, T.L. Hill, Addison Wiley.
4. The Liquid State, J.A. Pryde.
5. Significant Liquid Structures, H. Eyring and M.S. John.

SEMESTER IV

Inorganic Chemistry

SOS/C022	Laboratory Course- Inorg. IVA	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do two exercises of 18 marks each.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

I. Spectrophotometric Determinations

- Manganese/chromium/vanadium in steel sample.
- Nickle/molybdenum/tungsten/vanadium/uranium by extractive Spectrophotometric method.
- Fluoride/nitrite/phosphate.
- Iron-phenanthroline complex: Job's Method of continuous variation.
- Zirconium-alizarin Red-S complex: Mole-ratio method.
- Copper-ethylene diamine complex: Slope –ratio method.

II. Flame Photometric Determinations

- Sodium and Potassium when present together.
- Lithium/Calcium/barium/strontium.
- Cadmium and magnesium in tap water.

SOS/C023	Laboratory Course- Inorg. IVB	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do two exercises of 18 marks each.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

I. Nephelometric Determinations

- Sulphate
- Phosphate
- Silver

II. Chromatographic separations: Paper or TLC and determination of R_f values:

- Cadmium and Zinc.
- Silver, Lead and Mercury.
- Nickel, Magnesium, Cobalt and Zinc.

SOS/C024	Inorganic Polymers	L	T	P	C	MM
		3	0	0	3	100

Unit I

Inorganic polymer synthesis, step-growth and step condensation synthesis of metal containing polymers.

Unit II

Condensation of functionalised metal containing species, condensation through bridged ligand coordination, bridging ligand formation during condensation, synthesis of main group condensation polymer.

Unit III

Polycarboranes, polycarbosilanes, polythiocyanines, polysiloxanes.

Unit IV

Chain polymerisations, radical and cationic polymerisations.

Unit V

Inorganic polymer characterization, methods of characterizing average molecular masses.

Unit VI

Glass transition temperature measurement, spectroscopic characterization specific to inorganic polymers, use of NMR and EPR in characterization of inorganic polymers, use of electronic, vibrational, Mossbauer spectroscopies in characterization of inorganic polymers, visco-elasticity measurements. Crystallinity characterization.

Unit VII

Polymer elastomers, inorganic dental polymers, adhesives, inorganic high temperature fluids and lubricants.

Unit VIII

Inorganic polymer conductivity, metal containing polymers, metal containing polymers in non linear optics, luminescent inorganic polymers.

Books suggested

1. Inorganic and Organometallic Polymers, Ronald D. Archer, Wiley VCH, 2001.
2. Inorganic Polymers, J. E. Mark et al., Prentice Hall, 1992.

SOS/E009	Spectroscopy	L	T	P	C	MM
		3	0	0	3	100

Unit I**Electron Spin Resonance Spectroscopy**

Principle and theory, Kramer degeneracy, g factor, electron-nuclear coupling (hyperfine structure), line shape and width, Mc Connell relationship, endor and eldor, electron-electron coupling. Techniques of measurement, application of ESR to organic free radicals and to transitional metal complexes (having and unpaired electron) including biological systems.

Unit II

Nuclear Magnetic Resonance Spectroscopy

- (a). Chemical shift values for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, carboxylic acids, amines, amides), chemical exchange, effects of deuteration, Karplus curve-variation of coupling constant with dihedral angle.
- (b). **Carbon-13 NMR Spectroscopy**
General consideration, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl compound), coupling constants.
- (c). **Nuclear Quadrupole Resonance:** Principle, Theory and applications

Unit III

Mass Spectrometry

Principle and theory, fundamental mass equation, ionization methods, odd and even electron ions, base peak, isotopic ions, fragmentation patterns, Mc Lafferty rearrangement and RD cleavage, Instrumentation; ESIMS, various analyzers used in mass spectrometry, application of mass spectrometry to the structure elucidation of organic molecules

Unit IV

Photoelectron Spectroscopy

Basic principles, photoelectric effect, ionization process, Koopman's Theorem, photoelectron spectra of simple molecules, ESCA, chemical information from ESCA, Auger electron spectroscopy-basic idea.

Books Suggested

1. Physical Method for Chemistry, R.S. Drago, Saunders Company.
2. Structural Method in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Craddock, ELBS
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
4. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpuech and G.J. Martin, Heyden.
5. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
6. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
7. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
8. Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman, G.S. Kriz, Thompson Asia Pvt. Ltd., Singapore.
9. Electronic spectroscopy, D.N. Sathyanarayan, Universities Press.
10. Interpretation of Mass Spectra, F.W. McLafferty, University Science Books, California.

SOS/E010	Bioinorganic, Bioorganic, Biophysical Chemistry-II	L	T	P	C	MM
		3	0	0	3	100

Unit I

Bioinorganic Chemistry

1. Electron Transfer in Biology

Structure and function of metalloproteins in electron transport processes-cytochromes and iron-sulphur proteins, synthetic models.

2. Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

Unit II

Bioorganic Chemistry

1. Co-Enzyme Chemistry

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD, lipoic acid, vitamin B₁₂. Mechanisms of reactions catalyzed by the above cofactors.

2. Enzyme Models

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, crown ethers, cryptates. Cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes.

3. Biotechnological Applications of Enzymes

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, use of enzymes in food and drink industry, brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Unit III

Biophysical Chemistry

1. Statistical Mechanism in Biopolymers

Chain configuration of macromolecules, statistical distribution, end-to-end dimensions, calculation of average dimensions for various chain structures. Polypeptide and protein structures, introduction to protein folding problem.

2. Biopolymer Interactions, Thermodynamics of Biopolymer Solutions

Forces involved in biopolymer interactions. Electrostatic charge and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.

3. Biopolymers and their Molecular Weights

Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions.

Books Suggested

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Bioinorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.
4. Understanding Enzymes, Trevor Palmer, Prentice Hall.
5. Enzyme Chemistry: Impact and Applications, Ed. Colliins J Sucking, Chapman and Hall.
6. Enzymes Mechanism Ed, M.I. Page and A. Williams, Royal Society of Chemistry.
7. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.
8. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
9. Enzymatic Reaction Mechanism, C. Walsh, W.H. Freeman.
10. Enzymatic Structure and Mechanism, W.H. Freeman.
11. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
12. Biochemistry, L. Stryer, W.H. Freeman.
13. Biochemistry, J. David Rawn, Neil Patterson.
14. Biochemistry, Voet and Voet, John Wiley.

15. Outlines of Biochemistry, E.E. Conn and P.K. Stumpf, John Wiley.

16. Macromolecules: Structure and function, F. World, Prentice Hall.

SOS/E011	Photoinorganic Chemistry	L	T	P	C	MM
		3	0	0	3	100

Unit I

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 process, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes.

Unit II

Properties of Excited States

Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics-calculation of rates of radiative processes. Biomolecular deactivation-quenching.

Unit III

Excited States of Metal Complexes

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.

Unit IV

Ligand Field Photochemistry

Photosubstitution, photo oxidation and photo reduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

Unit V

Redox Reactions by Excited Metal Complexes

Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidizing character of Ruthenium²⁺, (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.

Unit VI

Metal Complex Sensitizers

Metal complex sensitizer, electron relay, metal colloid system, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

Books Suggested:

1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.
2. Inorganic Photochemistry, J. Chem. Educ., vol. 60, no. 10, 1983.
3. Progress in Inorganic Chemistry, vol. 30, ed. S.J. Lippard, Wiley.

4. Co-ordination Chem. Revs., 1975, 15, 321; 1981, vol. 39, 121, 131; 1990, 97, 313.
5. Photochemistry of Co-ordination Compounds, V. Balzari and V. Carassiti, Academic Press.
6. Elements of Inorganic Photochemistry, G.J. Ferraudi, Wiley.
7. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern.
8. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
9. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
10. Introductory Photochemistry, A. Cox

SOS/E012	Environmental Chemistry	L	T	P	C	MM
		3	0	0	3	100

Unit I

Environment

Introduction, composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O. Bio distribution of elements.

Unit II

Hydrosphere

Aquatic pollution- inorganic, organic, pesticides, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters-dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards. Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.) residual chloride and chlorine demand. Purification and treatment of water.

Unit III

Soils

Composition, micro and macro nutrients, Pollution of fertilizers, pesticides and metals.

Unit IV

Atmosphere

Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals chlorofluorohydrocarbons. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

Unit V

Industrial Pollution

Pollution from cement, sugar, distillery, drug; paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers and drugs etc.

Unit VI

Environmental Toxicology

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes.

Books suggested

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma and Kaur, Krishna Publishers.

- Environmental Chemistry, A.K. De, Wiley Eastern.
- Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern.
- Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
- Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
- Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
- Environmental Chemistry, C. Baird, W.H. Freeman.

Organic Chemistry

SOS/C025	Laboratory Course	L	T	P	C	MM
	Org.-IVA	0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do two exercises of 18 marks each.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

I. Extraction of Organic Compounds from Natural Sources

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

II. Paper Chromatography

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.

Books Suggested

- Introduction to Organic Laboratory Techniques (Third Edition), DL Pavia, GM Lampman and GS Kriz, Saunders College Publishing, Philadelphia, New York.
- Operational Organic Chemistry, A Laboratory Course, Second Edition, JW Lehman, Allyn & Bacon, Inc. Boston.
- Microscale Organic Experiments KL Willianson, DC Health & Co. Le Xington.
- Laboratory Manual of Organic Chemistry, RK Bansal, New Age International, Delhi.

SOS/C026	Laboratory Course	L	T	P	C	MM
	Org.-IVB	0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do two exercises of 18 marks each.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

I. Spectroscopy

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

II. Spectrophotometric (UV/VIS) Estimations

1. Amino acids
2. Proteins
3. Carbohydrates
4. Cholesterol
5. Ascorbic acid
6. Aspirin
7. Caffeine

Books Suggested

5. Introduction to Organic Laboratory Techniques (Third Edition), DL Pavia, GM Lampman and GS Kriz, Saunders College Publishing, Philadelphia, New York.
6. Operational Organic Chemistry, A Laboratory Course, Second Edition, JW Lehman, Allyn & Bacon, Inc. Boston.
7. Microscale Organic Experiments KL Willianson, DC Health & Co. Le Xington.
8. Laboratory Manual of Organic Chemistry, RK Bansal, New Age International, Delhi.

SOS/C027	Natural Products	L	T	P	C	MM
		3	0	0	3	100

Unit I

Terpenoids and Carotenoids

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule Structures of abietic acid and β -carotene.

Unit II

Alkaloids

Isolation, structure and synthesis of ephedrine, quinine.

Unit III

Steroids

Structure determination of cholesterol and bile acids (without synthesis). Chemistry of testosterone, estrone and progesterone.

Unit IV

Pigments

(a) **Plant Pigments:** Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of cyanidin, and quercetin.

(b) Porphyrins

General Introduction of haemoglobin and chlorophyll. Chemistry of chlorophyll (without synthesis). Structure and synthesis of haem.

Unit V

Prostaglandins

Occurrence, nomenclature, classification, biogenesis and physiological effects

Synthesis of Key intermediate, PGE₂ and PGF_{2α}

Books Suggested

1. Natural Products: Chemistry and Biological Significance, J.Mann, R.S. Davidson, J.B. Hobbs, D.V. Bantrophe and J.B. Harborne, Longman, Essex.
2. Organic Chemistry, Vol 2, I.L. Finar, ELBS.
3. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt. Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers.
7. New Trends in Natural product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers

SOS/E013	Heterocyclic Chemistry	L	T	P	C	MM
		3	0	0	3	100

Unit I

Nomenclature of Heterocycles

Replacement and Systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles

Unit II

Aromatic and Non-aromatic Heterocycles

General chemical behaviour of aromatic heterocycles, classification (structural type), Heteroaromatic reactivity and tautomerism in aromatic heterocycles

Strain –bond angle and torsional strains and their consequences in small ring heterocycles.

Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interactions.

Stereo-electronic effects, aromatic and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic, electrophilic interactions.

Unit III

Small Ring Heterocycles

Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes

Unit IV

Benzo-Fused Five-Membered Heterocycles

Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes

Unit V

Six-Membered Heterocycles with One, Two or More Heteroatoms

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones

Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones Synthesis and reactions of diazines, triazines, tetrazines and thiazines

Unit VI

Seven-and Large-Membered Heterocycles

Synthesis and reactions of azepines, oxepines, thiepinines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines

Books Suggested:

1. Heterocyclic Chemistry Vol. 1 & 2, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon
8. Natural Products: Chemistry and Biological Significance, J.Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrophe and J.B. Harborne, Longman, Essex.
9. Organic Chemistry, Vol 2, I.L. Finar, ELBS.
10. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH

Physical Chemistry

SOS/C028	Laboratory Course Phy.-IVA	L	T	P	C	MM
		0	0	9	3	100

Note: The duration of examination will be of eight hours spread over two days. Students are required to do two exercises of 18 marks each.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

1. Determination of transport number.
2. Determination of liquid junction potential.
3. Determination of the charge on colloidal particle.
4. Polarography.
5. Beer's law verification.

SOS/C029	Laboratory Course Phy.- IVB	L	T	P	C	MM
		0	0	9	3	1000

Note: The duration of examination will be of eight hours spread over two days. Students are required to do two exercises of 18 marks each.

Viva 09 marks

Seminar/Attendance/Assessment/Record 15 marks.

1. Decomposition of potential determination.
2. Validity of Freundlich's adsorption isotherm.
3. Validity of Langmuir's adsorption isotherm.
4. Determination of partial molar volume of solute.
5. Determination of CMC of surfactants.

SOS/C030	Advanced Quantum Chemistry	L	T	P	C	MM
		3	0	0	3	100

(Pre-requisite: mathematics at least up to First Year B.Sc. level is necessary. At least one PC among 4 students should be available)

Unit I

Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock Theory

Review of the principles of quantum mechanics, Born-Oppenheimer approximation. Slater-Condon rules, Hartree-Fock equation, Koopmans and Brillouin theories, Roothan equation, Gaussian basis sets.

Unit II

Configuration Interaction and MC-SCF

Introduction to CI; full and truncated CI theories, size consistency, Introductory treatment of coupled cluster and MC-SCF methods.

Unit III

Semi-Empirical Theories

A review of the Huckel, EHT and PPP treatments, ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An introduction to MOPAC and AMI with hands on experience on personal computer.

Unit IV

Density Functional Theory

Derivation of Hohenberg-Kohn theorem, Kohn-Sham formulation, N- and V- representabilities; review of the performance of the existing local (e.g. Slater X α and other methods) and non-local functionals, treatment of chemical concepts with the density functional theory.

Unit V

Computer Experiments

Computer experiments using quantum chemistry- software packages such as GAUSSIAN/GAMESS/MOPAC and modeling software e.g. MM2/ AMBER/ CHARM etc.

Books Suggested

1. Modern Quantum Chemistry, N.S. Ostlund and a. Szabo, McGraw Hill.
2. Methods of Molecular Quantum Mechanics, R. Mcweeny and B.T. Sutcliffe, Academic Press
3. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford.
4. Exploring Chemistry with Electron Structure Methods, J.B. Foresman and e. Frish, Goussian Inc.
5. Semi-empirical MO Theory, J. Pople and D.L. Beveridge.

SOS/E014	Polymers	L	T	P	C	MM
		3	0	0	3	100

Unit I

Basics

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain, ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions. Polymerization n homogenous and heterogeneous systems.

Unit II

Polymer Characterization

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation 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.

Unit III

Structure and Properties

Morphology and order in crystalline polymers, configurations of polymer chains. Crystal structure of 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, T_g . Relationship between T_m and T_g , effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

Unit IV

Polymer Processing

Plastic, elastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

Books Suggested

1. Textbook of Polymer Science, F.W. Billmeyer Jr, Wiley.
2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R.M. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
5. Physics and Chemistry of Polymers, J.M.G. Cowie, Blackie Academic and Professional.