

Unit-I Rotational Spectroscopy

Quantization of rotational energy and interactions of radiation with rotators. Classification of rotators; rigid rotator and Non-rigid rotator linear, symmetric and asymmetric rotators, isotopic effect, stark effect, effect of nuclear spin, and electron spin on rotational spectra, Bond length calculations.

Unit-II (A) Vibrational Spectroscopy

Harmonic oscillator model, harmonic and anharmonic vibration, Normal vibration, Factors affecting vibration frequencies, vibrating rotators, P,Q,R. Branches, overtones, anharmonicity constant, Raman effect, stokes and antistokes lines, selection rules for IR and Raman spectra, Principal of mutual exclusion. Polarization of Raman Lines.

Unit-III Photoelectron Spectroscopy

Basic principles of photoelectric effect, ionization process, Adiabatic and vertical ionization energy, PESOS(UV-PES) and PESIS (XPES or ESCA). Chemical shift in ESCA. Chemical information from ESCA. Instrument and Techniques of Photoelectron Spectroscopy. Atomic electron spectra of inert gases. Comparison of Photo-electron spectra of Ar, Kr, Xe. Photo-electron spectra of H_2 , O_2 , N_2 and NO, HBr. XPES or ESCA of Furan, Pyrrole and Thiophene. Zero kinetic energy. Photoelectron Spectroscopy. Auger Spectroscopy(AES). Scanning Auger Microprobes(SAM). Microscopic Technique : SEM, TEM, STEM, Focus ion beam Spectroscopy(FIB). Electron Microscope Koopman's theorem.

Unit-IV Magnetic Resonance Spectroscopy

Nuclear magnetic resonance, chemical shift of factors controlling its value spin-spin interaction and factors affecting its value. Spin Lattice relaxation and quantitative treatment of relaxation, selection rule and relative intensities of line. Principle of ESR spectroscopy, presentation of spectrum, theory of hyperfine, interaction, Isotopic g and Δ values.

Nuclear quadrupole resonance spectroscopy. Basic Concepts of NQR, Electric field gradient, NQR frequency for N^{14} ($I=1$) B^{11} ($I=3/2$), ^{27}Al ($I=5/2$). Nuclear quadrupole coupling constant.

Unit-V Applications of Spectroscopy

(A) UV-Visible Spectroscopy

Spectra of carbonyl compounds and conjugated polyenes, Woodward-Fisher rules, aromatic and heterocyclic compounds, and steric effect in diphenyls, quantitative determinations.

(B) Vibrational Spectroscopy

Organic effect of conjugation, resonance inductive effect, ring strain and hydrogen bonding on group frequencies and band shapes.

Inorganic: Changes with vibrational frequencies upon coordination, cases of linkage isomers, I.R. and Raman active form of vibrational geometry of AB_2 , AB_3 , AB_4 , and AB_5 . Hydrogen bonding.

(C) PMR and CMR Spectroscopy

Chemical shifts value and correlation for proton-bonded with carbon. Effect of chemical exchange on line width, coupling constants, Interpretation of PMR and CMR spectra of organic compounds. Double resonance application of ^{19}F and ^{31}P spectra of inorganic compounds.

(D) Mass Spectrometry Ion production and Fragmentation, molecular ion peak, Metastable peak, Mc. Lafferty rearrangement. Examples of mass spectra of organic compounds.

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Book Suggested Recommended:

1. Physical Methods for Chemistry by R.S. Drago, Saunders Company.
2. Structural Methods in Inorganic Chemistry by E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and Raman Spectra: Inorganic and Co-ordination pounds by K. Nakamoto, Wiley.
4. Progress in Inorganic Chemistry Vol. 8, ed by F.A. Cotton, Vol. 15, ed, S.J. Lipard, Wiley.
5. Inorganic Electronic Spectroscopy by A.P.B. Lever, Elsevier.
6. Organic Spectroscopy by Jagdamba Singh and Jaya Singh.
7. Spectroscopy of Organic Compounds by P S Kalsi.
8. Spectrometric identification of organic compounds by Silverstein.

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Semester -III
Core Course-XI
Bio-Inorganic Chemistry

Full Marks-70

Credits-5

Unit-I Metal Ions in Biological Systems

Essential and trace metals. Na^+/K^+ Pump, Role of metal ions in biological processes Toxicity of heavy metals and their detoxification, role of Selenium in Biological systems with reference to its essentiality and toxicity, mechanism of metal ion induced toxicity, interaction between orally administered drugs and metal ions in gut.

Unit-II Bioenergetics and ATP Cycle

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

Unit-III Transport and Storage of Dioxygen

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

Unit-IV Electron Transfer in Biology

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

Nitrogenase

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

Unit-V Metals in Enzyme and Medicine

The biochemistry of zinc, cobalt, nickel and molybdenum: Transport of Zinc, carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase, Adenosyl cobalamine as a coenzyme. Ribonucleotide reductase, Methylcobalamine and cyano cobalamine as a co-factor, Nickel in urease, Hydrogenase, Molybdenum hydroxylase, Xanthine oxidase, Sulphite oxidase, nitrate reductase.

Biochemical basis of essential metal deficient diseases, Iron copper and Zinc deficiency and their therapies, Carcinogens and carcinostatic agent, Zinc in tumors growth and inhibital anticancer activity and Mechanism of platinum, Rhodium, copper and Gold complexes.

Books Recommend:

1. Principles of Bio-inorganic Chemistry - S.J Lippard and J.M Berg, University Science Books.
2. Bio-inorganic Chemistry- I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine University Science Books
3. Progress in Inorganic Chemistry, Vols 18 and 35 Ed. J.J. - Lippard, Wiley.

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Semester-III
Core Course-XII

(Environmental Chemistry and Green Chemistry)

Full Marks-70

Credits-5

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

Chemicals compositions of water bodies-lakes, streams, rivers, and wet lands etc. hydrological cycle, Aquatic Pollution - inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters - dissolved oxygen, biochemical oxygen demand (BOD), Solids, metals, content of chloride, sulphate, phosphate, nitrate and microorganism. Water quality standards.

Analytical methods for measuring BOD, DO, COD, F, Oils, Metals (As, Cd, Cr, Hg, Pd, Se, etc.), Residual chloride and chlorine demand. Purification and treatment of waste water.

Unit-III Atmosphere

Chemical composition of atmosphere-particles, ions and radical and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effects, pollution by chemicals, petroleum, minerals, chlorofluorocarbons (CFC's). Greenhouse effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

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Unit-IV Green Chemistry: Definition and Objective

The twelve principles of Green Chemistry, atom economy in chemical synthesis, important techniques employed in practice of Green Chemistry, Application of microwave irradiation and ultrasound in chemical reactions. Use of renewable raw materials and biosynthesis, organic waste management, use of safer reagents green solvents and green catalysts.

Unit-IV Green Chemistry: Real Applications

Replacement of CFC and hydrocarbon blowing agents with environmental friendly blowing agent CO₂ in the production of polystyrene. Replacement of Ozone depleating and Smog producing solvents by surfactant assisted liquid or supercritical carbon dioxide for cleaning in manufacture of ICs and Computer chips.

Books Suggested

1. Environmental Chemistry and Green Chemistry, Asin Kr Das, Books and Allied (P) Ltd, Kolkata.
2. Environmental Chemistry, H. Kaur, Pragati Prakashan.
3. Environmental Chemistry S.F. Manahan, Lewis Publishers
4. Environmental Chemistry, A.K. Dey, Wiley Easlem.
5. Environmental Chemistry, C. Baird, W.H. Freeman.

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Semester-III
Core Course-XIII
(Bio- Organic Chemistry)

Full Marks-70

Credits-5

Unit-I Enzymes

Basic considerations, Proximity effects and Molecular adaption. Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity extraction and purification. Fischer's lock and key 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.

Unit-II Mechanism of Enzyme Action

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion, Examples of some typical enzyme mechanisms for chymotrypsin, lysozyme and carboxypeptidase A.

Unit-III Reactions Catalysed by Enzymes

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

Unit-IV Co-Enzyme Chemistry

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes, Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD, NADH, FMN,

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FAD, Lipole acid, vitamin B12, Mechanisms of reactions catalyzed by the above cofactors.

Unit-V Bioenergetics and Protein Metabolism

Free energy and entropy change in biochemical reactions. Synthesis of ATP. ATP as biological currency. Calvin cycle kerb cycle, glycolysis and glycogenesis. Amino acid metabolism, urea cycle. Chemical basis of heredity. Replication of DNA. Translation and Transcription.

Books Recommend:

1. Understanding Enzymes- Trevor Palmer, Prentice Hall.
2. Enzyme Chemistry - Impact and Application, Ed.- Collin J. Suckling, Chapma and Hall.
3. Enzyme Mechanisms Ed- M.J Page and A. Villiams, Royal Society of Chemistry.
4. Fundamentals of Enzymology- N.C. Price and L. Slovens, Oxford University Press.
5. Immobilized Enzymes- An Introduction and Applications in Biotechnology, Michael O. Trevan, John Wiley.
6. Enzymatic Reaction Mechanisms- C. Walsh, w.H. Freeman.
7. Enzyme structure and Mechanism- A. Fersht, W.H. Freeman.

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Semester-III
Core Course-XIV
Practical (Inorganic Chemistry)

Full Marks-50

Duration of Exam 6 hrs.

Credits-5

- Quantitative analysis of two constituent ions of the following.
(a) Cu, Zn, (b) Fe, Ni (c) Ca, Mg (d) Al, Mg the cations
Mg²⁺, Ca²⁺ and Al³⁺ can be estimated using EDTA. 15
- Green methods of preparation of the following complexes and their study
by IR, electronic spectra and T.G.A. 15
 - Pot trioxalato ferrate (III)
 - Pot trioxalato chromate(III)
 - Chromus Acetate
 - Hg[Co(SCN)₄]
 - Hexa ammine Ni (II) chloride
- Qualitative analysis of inorganic mixture containing six radicals including
interfering radicals 15
- Viva-voce 15
- Note Book 5

Books Recommend:

- A text Book of Quantitative Inorganic Analysis- A.I. Vogel
- Applied Analytical chemistry- O.P. Vermani

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Semester-III
AECC-2
Human values and professional ethics & gender sensitization

28/11/19

