Course No: CHM-301

Title: Bioinorganic Chemistry and Applications of Spectroscopy.

Max. Marks: *100* ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment:*** *20 Marks*
Total Duration: *(50 hrs.)*

Unit-I: Metal—Ions in Biological Systems: (12hrs)

Classification of elements in human systems. Concept of essentiality and evolution of essential elements.

Distribution and biological role of essential trace and ultra trace elements like V, Cr, Mn, Ni, P, and halogens.

Effects of deficiency of essential trace elements hi biological systems and its treatment. Antagonism and Synergism among essential trace elements.

Role of alkali and alkaline earth metal—ions hi biological systems and their mechanism of transport in cell membrane.

The Sodium / Potassium pump. Lithium and the mental health. Chlorophyll and its role in Photosynthesis.

Unit-II: Transport and Storage of Dioxygen. (12hrs)

Porphyrins: Introduction, Characteristic absorption spectrum and Salient features. Haemoglobin and Myoglobin: Structure , Bohr effect; Cooperative interaction in haemoglobin. Mechanism of oxygen transport in human body.

Hemerythrin and Hemocyanin: Structure , Metal binding groups and Dioxygen binding. Synthetic Oxygen Carriers : Vaskas iridium complex ; Cobalt complexes with micro--, and macrocyclic ligands; salen and acacen ligands.

Biological Nitrogen Fixation : Dinitrogen complexes and their reactivity ; Nitrogenase enzyme; fixation via nitride formation .

Unit-III: IR, Raman and EPR Spectroscopy. (16 hrs)

Symmetry of IR and Raman active normal vibrational modes of AB2, AB_3, AB_4 , AB_5, and ABe type molecules.

Metal Isotope Technique, Normal Coordinate Analysis (introductory idea).

Mode of bonding of ambidentate ligands: ethylenediamine and diketonato complexes. Raman Spectroscopy particularly for the study of active sites of Metalloproteins .

EPR : Hyperfine coupling, Fermi contact, Spin polarization effects, Dipolar coupling, Me Conell equation and calculation of spin densities hi inorganic radicals such as CO_2^- CH_3^-,BH_3^-andF_2- Spin orbit coupling and significance of g tensors.

Unit-IV: Mossbauer Spectroscopy. (l0hrs)

Basic principles, Spectral parameters such as isomer shift, quadrupole splitting and magnetic splitting, spectrum display.

Application of the technique to the studies of i)bonding and structure of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, ii) Sn^{2+} and Sn^{4+} compounds— nature of M—L bond, coordination number and structure, iii) detection of oxidation state and inequivalent MB atoms.

Books Recommended:

1. *The Inorganic Chemistry of Biological Processes; Huges; Wiley; 1973.*
2. *Bioinorganic Chemistry - An introduction ; Ochiai; Allyn and Bacon ; 1977.*
3. *Principles of Bioinorganic Chemistry; S.J. Lippard and J.M. Berg; University Science Books.*
4. *Inorganic Bio chemistry; Vols. I & II; G.L.Eichhorn ; Elsevier; 1973. '"*
5. *Physical Methods for Chemistry; 2nd edn., R.S.Drago ; Saunders ; 1992.*
6. *Structural Methods in Inorganic Chemistry; 2nd edn. E. A. V. Ebsworth & D.W.H. Rankin; ELBS; 1991.*
7. *Spectroscopy in Inorganic Chemistry; Vols I& II; Rao, Ferraro ; Academic;1970.*
8. *Infrared and Raman Spectra: Inorganic and Coordination compounds ; K. Nakamoto; Wiley.*
9. *NMR, NQR and Mossbauer Spectrascopy in Inorganic Chemistry ; R.V.Parish ;Ellis Horwood*

Course No: CHM-302
Title: Organic Chemistry

Max. Marks: *100* ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment:*** *20 Marks*
Total Duration: *(50 hrs.)*

Unit-I: Applications of Spectroscopy (Organic) and Photochemistry. (14 hrs)

Ultraviolet spectroscopy:

Ultraviolet absorption spectra of enones, dienes (homo and heteroannular) carbonyl compounds, aromatic and heteroaromatic compounds. Effect of conjugation on ultraviolet spectra, Woodward-Fieser rules, application and limitation. Kuhn's rule, application to conjugated polyenes.

Infrared Spectroscopy:

Introduction, instrumentation and sample handling, characteristic vibrational frequencies of hydrocarbons, alcohols, ethers , phenols,amines, aldehydes, ketones, acids, anhydrides, esters, lactones, amides and conjugated carbonyl compounds. Effect of hydrogen bonding on vibrational frequencies in IR spectra. Overtones, combination bands and Fermi resonance, FT-IR.

Mass Spectrometry:

Introduction, instrumentation, a typical mass spectra, molecular ion peak. Ion production, EI, CI, FD and FAB methods. Role of isotopes in mass spectrometry. Fragmentation pattern of various classes of organic compounds. Metastable peak, McLafferty rearrangement, nitrogen rule, high resolution mass spectrometery.

Unit-II: Nuclear magnetic resonance spectroscopy. (14 hrs)

General Introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercapto). Chemical exchange, effect of deuteration, complex spin-spin interactions between two three, four and five nuclei (first order spectra) virtual coupling, stereochemistry, hindered rotation Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effect. Fourier transform technique, nuclear overhauser effect (NOE)

Carbon-13 NMR Spectroscopy:

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromtic and carbonyl carbon), coupling constant.

Structure determination of organic compounds based on their spectral data (UV, IR, NMR and mass). Problem based exercises.

Unit-III: Photochemistry-I. (11hrs)

Photochemical Reactions

Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states and their lifetimes. The fate of excited molecule.(Physical and chemical processess). Transfer of excitation energy: Sensitization and Quenching, Quantum yield, types of photochemical reactions.

Photochemistry of alkenes

Geometrical isomerisations, cyclisation and dimerisation reactions. Photochemical reactions of 1,3- butadiene (excluding pericyclic reactions). Rearrangement of 1,4 and 1,5- dienes.

Photochemistry of saturated carbonyl compounds

Intramolecular reactions of saturated acyclic and cyclic carbonyl compounds. (Norrish type-I and Norrish type-II processess). Intermolecular cycloaddition reactions (Paterno- Buchi reaction).

Unit-IV: Photochemistry –II. (11 hrs)

Photochemistry of unsaturated carbonyl compounds

Photochemical reactions of α, β-unsaturated carbonyl compounds. (H-Abstraction and isomerisation to β, γ-unsaturated carbonyl compounds). Photolysis of cyclic α, β- unsaturated ketones (dimerisation and lumiketone rearrangement) and cyclohexadienones.

Photochemistry of Aromatic compounds

Photoinduced isomerisations of benzene and its alkyl derivatives. 1,2 ; 1,3 and 1,4 photoaddition reactions of benzene. Nueleophilic photosubstitution reactions in aromatic compounds. Photo Fries-rearrangement of aryl esters and anilides.

Miscellaneous Photochemical reaction

Photolysis of organic nitrites and their synthetic utility (Barton reaction).

Photochemistry of vision.

Books recommened:

1. *Spectrometric identification of Organic Compounds. 5th Ed., R.M.Silverstein, G.C.Bassler and T.C.Morill. (Jhon Wiley-1991).*
2. *Introduction to NMR Spectroscopy, R.J.Abraham. J.Fisher and P.Loftus (Wiley-1991)*
3. *Applications of absorption spectroscopy of Organic Compounds, J.R.Dyer (Prentice Hall-1991).*
4. *Spectroscopic Methods in organic Chemistry, D.H.Williams; I.Fleming (Tata-McGraw Hill-1988).*
5. *Intoductory Photochemistry, A.Cox and T.Kemp (McGraw Hall-1971).*
6. *Organic Photochemistry, 2nd Ed., J.Coxon, and B.Halton (2nd Ed. Cambridge University press-1987).*
7. *Fundamentals of photochemistry, Rohtagi & Mukherjee (Wiley Eastern-1992).*

Course No: CHM-303
Title: Physical Chemistry

Max. Marks: *100* ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment:*** *20 Marks*
Total Duration: *(50 hrs.)*

Unit-I: Irreversible Thermodynamics. (12 hrs)

Irreversible processes and uncompensated heat, degree of advancement, reaction rate & affinity. Gibb's equation, entropy production, entropy production due to matter flow, heat flow, charge flow & chemical reactions.

Concept of forces & fluxes, Onsagers theory of irreversible processes- phenomenological laws, their domain of validity. Chemical reactions near equilibrium. Transformation properties of forces and fluxes. Electrokinetic phenomena.

Unit-II: Crystal defects and solid state reactions. (12 hrs)

Various classifications of crystal defects. Thermodynamics of Schottky & Frankel defects.

Dislocations- their types. Colour centers.

Solid state reactions - general principles. Experimental procedures. Kinetics of Solid-state reactions (Solid-Solid & Solid-Gas reactions)

Unit-III: Electronic Properties & Band Theory. (13 hrs)

Free electron theory of metallic solids, Band theory of solids.

Semiconductors- Intrinsic & extrinsic semiconductor (n-type & p-type). Doping semiconductors, p-n junction. Super conductors- characteristic properties and applications.

Magnetic properties of solids: origin of magnetism in solids, Diamagnetism, paramagnetism – ferromagnetism, antiferromagnetism and ferrimagnetism. Temperature dependence of magnetization.

Unit-IV: Surface Chemistry. (13 hrs)

Pressure difference across curved surfaces (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET equation and its use in estimation of surface area, catalytic activity at surfaces.

Determination of molecular mass of colloidal particles through-Sedimentation, Viscosity and light scattering methods.

Hydrophobic interactions, Micellization, factors affecting the Micellization, Thermodynamics of micellization - phase separation and mass action models, Regular solution theory for mixed micellization.

Books Recommended:

1. *Physical Chemistry for the Chemical and Biological Sciences, R. Chang, University Science Books, 2000.*
2. *Concepts in Biochemistry, R. Boyer, Brroks/Cole Publishing Company, 1999.*
3. *Fundamentals of Biochemistry, D. Voet, J. G. Voet, C.W. Pralt, Wiley, 1999.*
4. *Lehninger Principles of Biochemistry, D.L. Nelson, N. M. Cox, Worth publishers, 2000.*
5. *Thermodynamics of Irreversible Processes, De Groot, North-Holland, 1966.*
6. *Introduction to Thermodynamics of Irreversible Processes, I. Prigogine, Interscience, 1967.*
7. *Molecular Thermodynamics, D. A. McQuarrie, J. D. Simon, Univ. Sci. Books, 1999.*
8. *Exploring Complexity, I. Prigogine, G. Nicolis, Freeman, 1998.*
9. *Introduction to Solids, Azaroff, Tata McGraw,1993.*
10. *Solid State Chemistry and its Applications, West, Wiley,1989.*
11. *The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.*
12. *Solid State Reactions, Schmalzried, Academic press, 1995.*
13. *Solid State Physics, N.W.Ashcroft and N.D.Mermin, Saunders college, 2001*

Course No: CHM-304
Title: Environmental Chemistry

Max. Marks: *100* ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment:*** *20 Marks*
Total Duration: *(50 hrs.)*

Unit –I: Environment and Soils. (12 hrs)

Introduction, Segments of Environment; factors affecting Environment. Biogeochemical cycles of C, N, P, S and O.

Nature and Composition of Soil: Air, Water, Inorganic Components, Organic matter and Humus. Macro and Micronutrients in Soil. Acid--Base and Ion exchange reactions in Soil.

Pollution: Fertilizers, Pesticides, Plastics and Metals.

Unit-II: Hydrosphere: (12 hrs)

Chemical composition of water bodies: - Lakes & rivers ; Factors determining composition (thermal stratification, acid-base, pE concept).

Aquatic pollution: Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage. Water quality parameters: Dissolved oxygen, Metals, Content of Chloride, Phosphate, Nitrate, and Microorganisms. Water quality standards.

Analytical Methods for determining BOD, DO, COD, and metals (As, Cd, Hg, Pb & Se) Choice of methods for determination.

Purification and treatment of water (Chlorination, Ozonation, UV radiation)

Unit-III: Atmosphere. (12hrs)

Chemical Composition of Atmosphere: particles, ions, radicals and their formation. Vertical profile of atmosphere, Heat budget of earth s atmospheric system. Chemical and Photochemical Reactions in Atmosphere, Photochemical Smog formation; Oxides of N, C, S and their effects, Sun screens ; Ozone chemistry. Pollution by Chemicals (cholorofluorocarbons, hydrocarbons, 03)

Green House Effect; Acid Rain; their chemistry and control, Atmospheric Window. Analytical Methods for measuring Air Pollutants.

Continuous monitoring instruments.

Unit —IV: Environmental Toxicology and Industrial Pollution. (14 hrs)

Principles of Toxicology ; Dose Response Relationship ; Risk assessment and management.

Organochlorine Compounds: Accumulation and fate in biological systems. Toxicology of PCBs, Dioxins and Furans; Health effects in humans.

Environmental Estrogens.

Industrial Pollution: - Cement, Sugar, Drug, Paper and pulp. Thermal power plants, Nuclear power plants and Polymers

Radio nuclide analysis: Disposal of wastes and their management..

Books Recommended:

1. *Environmental Chemistry; Nigel.J.Bunce; Wurez Publishers; 1991.*
2. *Environmental Chemistry; 2nd edn; Colin Baird; Freeman &Co; 1991.*
3. *A Textbook of Environmental Chemistry; O.D.Tyagi & M.Mehra; Anmol Publishers; 1990.*
4. *Environmental Chemistry; A.K.De; Wiley Eastern;1995.*
5. *Environmental pollution Analysis; S.M.Khopkar; Wiley Eastern.*
6. *Environmental pollution; B.K.Sharma& H.Kaur; Goel Publishcrs;1996.*
7. *Environmental Toxicology; Ed.Rose; Gordon & Breach Science Publishers.*
8. *Environmental Chemistry; S.E.Manahan; Lewis Publishers;2000*

Course No: CHM-305
Title: Computers for Chemists

Max. Marks: *50* ***Min. Qualifying Marks:*** *40%*
External Exam: *30 Marks.* ***Internal Assessment:*** *10 Marks*
Labwork: *10 Marks.* ***Total Duration:*** *(50 hrs)*

Unit-I: Introduction to Computers. (6 hrs: Theory + Lab)

Introduction to digital computers, brief history of computers, physical organization. Overview of Input, Output and Storage devices. Software: System and Application Softwares. Programming concepts, Flow charts, Algorithms. Elementary data types.

Unit-II: Fortran Programming-I. (8 hrs)

Fortan character set, Data Types (Integer, Real, Complex, Logical, Character); operators; assignments and expressions; Type specification statements. List directed input and output statements; the Implicit None statement. Programme examples.

Arrays: one-dimensional, declaring and initializing one-dimensional arrays, Examples. Two-dimensional or Rank-2 arrays, multi –dimensional or rank-n arrays

Unit-III: Fortran Programming - II (8 hrs)

Control transfer statements: Logical IF and Block-IF statements: Block-DO and Count control Do loops ; Nested IF and DO Blocks , Case Construct.

FORMATS and Formatted Write statements. FORMAT descriptors; the I, F, E, L, A Descriptors and their use in Output statements. The x, t and / descriptors.

An introduction to Files and File processing

Unit-IV: Programming in Chemistry (8 hrs)

Development of small computer codes involving simple formulae in chemistry such as van der Waals' equation, pH titration, kinetics, radioactive decay. Solution of linear simultaneous equations.

Lab Work (20 hrs)

Laboratory work based on Units II, III & IV (Extra time to be allotted for this)

Books Recommended:

1. *Fortran 77, Jain & Suri, (TMH, 1997)*
2. *Computer Programming in Fortran 90 and 95, Rajaraman , (PHI, 2002)*
3. *Introduction to Fortran 90/95, S. J. Chapman (TMH, 1999)*
4. *Fortran 90/95 Explained, Metcalf and Reid, (OUP, 1997)*
5. *Computer Software Applications in Chemistry - P. C. Jurs, John Wiley, 1996.*

Note: The Course will be of 50 marks out of which 10 marks are reserved for Internal Assessment. The distribution of marks out of 40 will be 30 marks for theory and 10 marks for Labwork.

Course No: CHM-306L
Title: Lab. Course in Physical Chemistry

Max. Marks: *150* ***Min. Qualifying Marks:*** *40%*
External Exam: *120 Marks.* ***Internal Assessment:*** *30 Marks*
Total Duration: *(150 hrs.)*

A. Conductometry.

1. Determination of the composition of a mixture of HCl and CH_3COOH by titration with standard NaOH.
2. Determination of degree of dissociation of a weak acid.

B. Potentiometry.

1. Determination of strength of an acid by titration with an alkali using quinhydrone electrode.
2. Titration of Fe (II) vs $K_2Cr_2O_7$ and determination of standard redox potential of Fe^{2+}/Fe^{3+}.

C. pH-metry.

1. Determination of strength and pK value of a weak acid by titration with an alkali.
2. Determination of degree of hydrolysis of aniline hydrochloride.

D. Polarimetry.

1. Determination of the specific rotation of an optically active compound and determination of unknown concentration from the calibration curve.
2. Determination of the rate constant of inversion of cane sugar catalysed be HCl.

E. Phase Equilibria.

1. Determination of the transition temperature of a solid.
2. Study of the phenol / water and carbon disulphide / methanol system.

F. Refractometry.

1. Determination of refractive index of some liquids and finding the composition of a binary liquid mixture by refractivity method.
2. Determination of molar refraction, molar polarisation and electron polarisability of liquids.

G. Calorimetry.

1. Determination of heat of neutralisation of a strong acid with a strong base.
2. Determination of heat of neutralisation of a weak acid with a strong base.

H. Spectrophotometry.

1. Establishing the validity of Beer-Lambert law.

2. Determination of composition of a binary mixture of $K_2Cr_2O_7$ and $KMnO_4$.

I. Chemical Kinetics.

1. Study of kinetics of hydrolysis of an ester catalysed by dil. HCl.
2. Determination of order of reaction between $K_2S_2O_8$ and KI by Initial rates method.

J. Viscometry.

1. Investigation of variation of viscosity with conc. and determination of unknown concentration.
2. Determination of the radius of a molecule by viscosity measurement.

Books Recommended:

1. Practical Physical Chemistry, Findley, Kitchener, Longman,1977.
2. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.