Course No: CHM-301

Title: Bioinorganic Chemistry, Organometallics and Inorganic 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: (12 hours)

The role of metal-ions in Metal-Protein systems: In trigger and control mechanisms; in a structural context; as Lewis acid and as redox catalysts.

Biodistribution and biochemical role of essential trace and ultra-trace elements:- Fe, Zn, Cu, V, Cr, Mn, Ni, P, F and I. Effects of their deficiencies and treatment.

Antagonism and Synergism among essential trace elements.

Alkali and Alkaline earth metal ions (Na^+, K^+, Ca^{2+} & Mg^{2+} Biological role; ligands and mechanism of ion transport (Facilitated transport, Carriers, Channeling and active transport of Cations).

Role of Lithium in mental health.

Chlorophyll: Structure and role of magnesium in photosynthesis.

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

Unit-II: Organometallic Compounds: (13 hours)

Introduction, History and Importance of organometallic compounds as reagents, additives and Catalysts.

Nomenclature and Classification of Organometallic compounds.

Effective atomic number (18-Valance electron) rule and its significance.

Stability of Organometallic Compounds towards heat, oxidation and hydrolysis.

Preparation, Properties, Structure, bonding and applications of Alkyls and aryls of Li, B and Al.

Synthesis, Structure and bonding in Zeise's Salt.

Homogenous Catalysis using Organometallic Compounds: Catalysis, Terminology of Catalysis and Tolman Catalytic loop;

Hydrogenation and Hydroformation reactions in alkenes.

Unit-III: (12 hours)

Applicaions of group theory to IR and Raman spectroscopy:- Symmetry of IR and Raman active normal vibrational modes of AB2, AB3, AB4 , AB5, and ABe type molecules.

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

Mode of bonding of ambidentate ligands: ethylenediamine and diketonato complexes.

Applications of Resonance Raman Spectroscopy in the study of vibrational modes of Metalloproteins .

Advanced concepts in EPR: Epr spectra of transition metal complexes. Hyperfine coupling, Fermi contact interaction, Dipolar coupling Spin orbit coupling and. anisotropy in g tensors. Interpretation of g-values Zero field splitting and Kramer's degeneracy. Interpretation of spectra.

Unit-IV: (l3 hours)

Mossbauer Spectroscopy: 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 Fe2+ and Fe3+ compounds including those of intermediate spin, (ii) Sn2+ and Sn4+ compounds— nature of M—L bond, coordination number and structure, (iii) detection of oxidation state and inequivalent MB atoms.

Nuclear Quadrupole Resonance spectroscopy: NQR isotopes, Nuclear quadruple moment; Electric field gradient; nuclear quadruple coupling constant; Effect of applied magnetic field, Applications.

Books Recommended:

1. Bioinrognaic Chemistry- An introduction; Ochiai; Allyn and Bacon; 1977.
2. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg; University Science Books; 1994.
3. The Inorganic Chemistry of Biological Processes; IInd edn.; M. N. Hughes; John Wiley; 1973.
4. Bioinorganic Chemistry- A Short Course; R. M. Roat- Malone; Wiley Interscience; 2003.
5. The Organometallic Chemistry of the Transition Metals; IInd edn.; R. H. Crabtree; John Wiley; 1994.
6. Principles of Organo-Metallic Chemistry; IInd edn.; P. Powell; Chapman and Hall; 1988.
7. Organometallic Chemistry- A unified Approach; IInd edn.; R. C. Mehrotra & A. Singh; New Age International; 2003.
8. Fundamental Transition Metal Organometallic Chemistry; Charles M. Lukehart; Brooks; 1985.
9. Basic Organometallic Chemistry- Concepts, Syntheses and Applications; B. D. Gupta adn A. J. Elias; University Press; 2010.
10. Physical Methods for Chemistry; 2nd edn., R.S.Drago ; Saunders ; 1992.
11. Structural Methods in Inorganic Chemistry; 2nd edn. E. A. V. Ebsworth & D.W.H. Rankin; ELBS; 1991.
12. Spectroscopy in Inorganic Chemistry; Vols I& II; Rao, Ferraro; Academic;1970.
13. Infrared and Raman Spectra: Inorganic and Coordination compounds ; K. Nakamoto; Wiley.
14. 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: (14 hrs)

Recapitulation of UV, IR Spectroscopy, Woodward-Fieser rule Characteristic absorptions of various functional groups. Interpretation of IR Spectra.

Mass Spectrometry: Introduction, instrumentation, Ionization methods like EI, CI, SIMS, FAB, MALDI, ESI, MS/MS. Mass Analyzers like Magnetic Sector Mass Analyzer, Double Focusing Mass Analyzer, Quadrupole Mass Analyzer, Time-of-Flight. Mass Analyzer Determination of Molecular Formula, Role of Isotopes, Nitrogen Rule, Metastable Peak. Fragmentation pattern like Stevenson rule , initial ionization event, α-cleavage, inductive cleavage, two bond cleavage, Retro-Diels. Alder cleavage, McLaffertey Rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, Carboxylic acids, Amines, Problems based on Mass Spectroscopy. Some specific examples from natural products like flavanoids terpenes, steroids, alkaloids.

Unit - II Nuclear Magnetic Resonance Spectroscopy: (14 hrs)

Basic concepts, Mechanism of Measurements, Chemical shift values for various classes of compounds. Fourier Transform (FT) , Techniques and advantages, Nuclear OVERHAUSER effect (NOE). One bond coupling, two bond coupling, three bond coupling, second order spectra A_2, AB, AX, AB_2, AX_2, A_2B_2. Proton exchange, deuterium exchange, Peak broadening exchange

C-13 NMR : Carbon 13-chemical shifts , proton coupled and decoupled spectra. Nuclear overhouser, Effect, Off-Resonance De-coupling, A quick dip in to DEPT-45 , DEPT-90, DEPT-135.

Introduction to two-dimensional spectroscopy methods, Cosy techniques, HETCOR technique, OESY, combined structure problems.

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 processes). 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: Quantum Chemistry-I (13 hrs)

Approximation methods

The Variation theorem, linear variation principle, application to hydrogen atom and helium atom. Perturbation theory -first order(non-degenerate & degenerate). Application of perturbation method to helium atom. (4 hrs)

Chemical Bonding

LCAO-MO approximation, H2+ molecular ion, brief introduction to H2. Molecular term symbols. Valence bond treatment of H2, comparison of MO and VB methods in the light of H2 molecule. Hybridization of orbitals (sp, sp2 &sp3). (6 hrs)

Huckel's Pi-MO theory: Application to linear and cyclic polyenes. Pi-electron charge and bond-order. (3 hrs)

Unit-II: Quantum Chemistry-II (12 hrs)

Huckel approximation continued: Alternant hydrocarbons, Naphthalene, heteroatomic conjugated systems. Limitations of Huckel theory. Parisar-Parr-Pople method, Extended Huckel Method. (5 hrs)

Self consistent field method: Hamiltonian and wave function for multi-electron systems. Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree and Hartree-Fock self consistent field methods. One and two-electron integrals in the light of minimal basis H_2 system. He atom. (7 hrs)

Unit-III: Electrochemistry-I (Ionics) (13 hrs)

Ion solvent Interactions: Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) treatments of ion-solvent interactions.

Ion-Ion Interactions: Activity and activity co-efficients. Debye-Huckel theory of activity coefficients of electrolyte solutions; derivation of Debye-Huckel limiting law, validity and extension to high concentrations; ion-pair formation-Bjerrum model. Debye-Huckel-Onsager conductance equation and brief idea of its extension.

Unit-IV: Electrochemistry-II (Interfaces) (13hrs)

Metal-electrolyte electrified interfaces, concept of surface excess, thermodynamics of electrified interface, Lippman equation, electrocapillary curves. Methods for determination of surface excess.

Structural models of metal-electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern models, recent advances. Semiconductor electrodes: Structure of seminconductor/electrolyte interface

Theories of Heterogeneous Electron Transfer: Electron transfer at electrified interface at and away from equilibrium. Butller-Volmer equation, low and high field approximations, significance of transfer coefficient.

Books Recommended:

1. Physical Chemistry - P. W. Atkins, ELBS , Oxford, 1997.
2. Physical Chemistry- A Molecular Approach - D. A. McQuarie & J. D. Simon, University Science Books, 1997.
3. Introduction to Quantum chemistry - A. K. Chandra, TataMcGraw Hill, 1997.
4. Quantum Chemistry - Ira. N. Levine, Prentice Hall, 2000.
5. Quantum Chemistry, Prasad, New Age Publishers, 2000.
6. Molecular Thermodynamics of Electrolyte Solutions, Lioyd L Lee, World Scientific, 2008.
7. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
8. Modern Electrochemistry 1, 2A, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
9. Electrochemical methods, Fundamentals and Methods, A.J. Bard, L.R. Faulkner, Wiley, 1980.
10. Physical Electrochemistry- Fundamentals, Techniques and Applications, Eliezer Gileadi, Wiley-VCH 2011.
11. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.

Course No: CHM-304
Title: Computers for Chemists

Max. Marks: *100* ***Min. Qualifying Marks:*** *40%*
External Exam: *60 Marks.* ***Internal Assessment:*** *20 Marks*
Labwork: *20 Marks.* ***Total Duration:*** *(50 hrs)*

Unit-I: (12 hrs)

Introduction to Computers (5 hrs)

Introduction to digital computers and their physical organization. Overview of Input, Output and Storage devices. Software: System and Application Softwares. Flow charts, Algorithms.

Fortran Programming - I (5 hrs)

Fortran character set, Intrinsic data types (Integer, Real, Complex, Logical, Character); kind specification. Operators, assignments and expressions; type specification statements. List directed input and output statements; the Implicit none & parameter statements. Program examples.

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

Unit-II: Fortran Programming - II (12 hrs)

Control transfer Structures: Logical IF and Block-IF statements, example programs; Block-DO and Count control DO loops, Nested IF and DO Blocks, Implied DO, Case Construct, example programs. **(4 hrs)**

Formated Input/Output: Formatted Read/Write statements. Format descriptors; the I, F, E, Es, L, and A descriptors and their use in Output statements. The x, t and / descriptors.

An introduction to Files and File processing. **(4 hrs)**

Development of small computer codes involving simple formulae in chemistry such as kinetics, radioactive decay, van der Waals' equation, pH titration. **(4 hrs)**

Unit-III: Advanced Features of Fortran 90/95 (12 hrs)

Derived data types. Program units and procedures: Function and subroutine subprograms, Passing character strings and arrays as dummy arguments, Functions & subroutines as dummy arguments, recursive functions.

Modules, Interface Blocks. Dynamic storage allocation; Where and Forall statements/constructs. Namelist Input/output

Unit-IV: Use of Computer packages (13 Hrs)

The students will learn how to run standard computer packages: (i) Microcal Origin / MS Excel (ii) Chemoffice, (iii) Mathematica.

X-Y plots, execution of linear and polynomial regression, numerical integration and differentiation, and solution of differential equations.

Lab Work **(30 hrs)**

Laboratory work based on Units I, 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. Fortran 90/95 for Scientists and Engineers, Stefan J Chapmann (TMH, 2005)
4. Fortran 90/95 Explained, Metcalf and Reid, (OUP, 1997)
5. Computer Software Applications in Chemistry - P. C. Jurs, (Wiley, 1996).
6. Excel for Chemists, A comprehensive Guide, E. Billo (Wiley, 2007)
7. Excel, Origin, ChemOffice and Mathemaitica manuals

Course No: CHM-305
Title: Industrial Pollution and Green Chemistry.

Max. Marks: *50* ***Min. Qualifying Marks:*** *40%*
External Exam: *40 Marks.* ***Internal Assessment:*** *10 Marks*
Total Duration: *(25 hrs)*

Unit-I: Industrial Pollution. (05 hours)

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.

Unit-II: Environmental Toxicology (07 hours)

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.

Unit-III: Green Chemistry-Theory (06 hours)

Introduction: Need for Green Chemistry and the role of chemists. Principles of Green Chemistry.

Tools of Green Chemistry:- Selection of starting materials, Catalysts, Alternative Solvents, Appropriate reagents, Percentage atom utilization. Microwaves and Sonication.

Unit-IV: Green Chemistry-Practice (07 hours)

Green Solvents and Reaction conditions: Supracritical fluids, Aqueous reaction conditions, Immobilized Solvents and irradiative reaction conditions.

Examples of Green materials, reagents and some specific reactions.

Books Recommended:

1. Environmental Chemistry; 8^{th} edn.; S. E. Manahan; CRC Press; 2005.

2. Chemistry of the Environment; IInd edn.; T. G. Spiro and W. M. Stigliani; Prentice Hall; 2002.

3. Environmental Chemistry; IInd edn.; Colin Baird; Freeman & Co.; 1991.

4. Chemistry of the Environment; IInd Edn. R. A. Bailey; H. M. Clark; J. P. Ferris; S. Krause & R. L. Strong; Elsevier; 2005.

5. Environmental Chemistry; IInd edn.; Samir K. Banergi; Prentice- Hall; 2001.

6. Green Chemistry- Environment Friendly Alternatives; Rashmi Sanghi & M. M Srivastava; Narosa; 2007.

7. Green Chemistry- An Introductory Text; IInd Edn.; Mike Lancaster; RSC; 2010.

8. Green Chemistry- Theory and Practice; P. T. Anastas and J. C. Warner; oxford; 2000.

9. Green Chemistry; Ist Edn.; Samuel Delvin; IVY Publishing House; 2008.

10. Green Chemistry- Environmentally Benign Reactions; V. K. Ahluwalia; Ane Books; 2006.

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. Determination of pKa value of a weak acid through potentiometry.
3. Titration of Fe (II) vs K2Cr2O7 and determination of standard redox potential of Fe^{2+}/Fe^{3+}.

C. pH-metry

1. Determination of strength and pKa value of a weak acid by titration with an alkali.
2. Titration of a tribasic acid with alkali to find its pKa values.
3. 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. 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.

F. Spectrophotometry

1. Establishing the validity of Beer-Lambert law.
2. Determination of composition of a binary mixture through spectrophotometry.
3. Spectrophotometric titration of Fe(II) vs $KMnO_4$

G. Chemical Kinetics

1. Determination of order of reaction between K2S2O8 and KI by Initial rates method.
2. Study of effect of temperature and ionic strength on rate constant of persulphate-iodide reaction.

H. Viscometry

1. Investigation of variation of viscosity with conc. and determination of unknown concentration.
2. Estimation of molecular radius of a solute using viscometry.

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.
4. Experimental Physical Chemistry,Arthur M. Halpern, George C. McBane, Freeman,2006.
5. Chemistry Experiments for Instrumental Methods, Sawyer, Heineman, Beebe, Wiley, 1984