Course No: CH14301CR
Title: Applications of Spectroscopy & Photochemistry (04 Credits)

Max. Marks: 100
Duration: 64 Contact hours
External Exam: 80 Marks.
Internal Assessment: 20 Marks

Unit-I: Applications of Spectroscopy: (16 Contact hours)
Recapitulation of UV, IR Spectroscopy, Woodward-Fieser rule Characteristic absorptions of various functional groups. Interpretation of IR Spectra.

Unit-II Nuclear Magnetic Resonance Spectroscopy: (16 Contact hours)
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 A2, AB, AX, AB2, AX2, A2B2. Proton exchange, deuterium exchange, Peak broadening exchange
Introduction to two-dimensional spectroscopy methods, Cosy techniques, HETCOR technique, OESY, combined structure problems.

Unit-III: Photochemistry-I. (16 Contact hours)
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 processes). Intermolecular cycloaddition reactions (Paterno- Buchi reaction).

**Unit-IV: Photochemistry –II.**

(16 Contact hours)

**Photochemistry of unsaturated carbonyl compounds**
Photochemical reactions of \(\alpha, \beta\)-unsaturated carbonyl compounds. (H-Abstraction and isomerisation to \(\beta, \gamma\)-unsaturated carbonyl compounds). Photolysis of cyclic \(\alpha, \beta\)-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. Nucleophilic 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 recommended:**

Course No: CH14302CR  
Title: Physical Chemistry.  (04 Credits)

Max. Marks: 100  
External Exam: 80 Marks.  
Duration: 64 Contact hours  
Internal Assessment: 20 Marks

Unit-I: Quantum Chemistry-I  
(16 Contact hours)

Approximation methods

Unit-II: Quantum Chemistry-II  
(16 Contact hours)
Chemical Bonding
Huckel's Pi-MO theory: Application to linear and cyclic polyenes. Pi-electron charge and bond-order.


Unit-III: Electrochemistry-I (Ionics)  
(16 Contact hours)
Ion solvent Interactions: Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) treatments of ion-solvent interactions.


Unit-IV: Electrochemistry-II (Interfaces)  
(16 Contact hours)
Metal-electrolyte electrified interface, 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 semiconductor/electrolyte interface

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

Books Recommended:

6. Coulson's Valence, R. Mcweeny, ELBS.
Course No: CH14303CR
Title: Laboratory Course in Physical Chemistry-1  (04 Credits)

Max. Marks: 100  Duration: 64 Contact hours
External Exam: 80 Marks.  Internal Assessment: 20 Marks

A. 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 by HCl.

B. 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.
   3. Determine the integral heat of solution of KNO₃.

C. Chemical Kinetics
   1. Study of kinetics of hydrolysis of an ester catalysed by dil. HCl.
   2. Determination of order of reaction between K₂S₂O₈ and KI by Initial rates method.
   3. Study of effect of temperature and ionic strength on rate constant of persulphate-iodide
      reaction.

D. 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:
   4. Experimental Physical Chemistry, Arthur M. Halpern, George C. McBane,
      Freeman, 2006.
   5. Chemistry Experiments for Instrumental Methods, Sawyer, Heineman, Beebe, Wiley,
      1984
Course No: CH14304EA
Title: Selected Topics in Chemistry. (04 Credits)

Max. Marks: 100
External Exam: 80 Marks.
Duration: 64 Contact hours
Internal Assessment: 20 Marks

Unit-I: Magnetic Properties and Electronic Spectra of Transition Metal Complexes. (16 Contact hours)

Types of magnetic behaviour, magnetic susceptibility and magnetic moment; methods of determining magnetic susceptibility; spin-only formula; L-S coupling, correlation of $\mu_s$ and $\mu_{\text{eff}}$ values; orbital contribution to magnetic moments; applications of magnetic moment data in investigation of nature of bonding and stereochemistry of first row transition metal complexes. High spin- low spin crossover.

Electronic spectra of Transition metal complexes: General features; Types of electronic transitions, theoretical aspects of d-d spectra, selection rules; spectral terms of $d^1 - d^{10}$ metal ions.

Selected examples of d-d spectra. Spectra of distorted octahedral and square planar complexes. Charge transfer spectra.

Unit-II: Metal-ions in Biological Systems: (16 Contact 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.


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-III: Applications of group theory to IR and Raman spectroscopy.  

(16 Contact hours)

Revision of group theory: Groups, subgroups, classes.
Symmetry elements and operations; combination of symmetry operations .Symmetry point groups, Matrix representation of symmetry operation. Representation, character of a representation,
Symmetry of IR and Raman active normal vibrational modes of AB2, AB3, AB4 , AB5,and AB6 type molecules.
Normal Coordinate Analysis (introductory idea).

Unit-IV: NQR & Mossbauer Spectroscopy.  

(16 Contact hours)

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

Books Recommended:

1. Bioinorganic Chemistry- An introduction; Ochiai; Allyn and Bacon; 1977.
10. Infrared and Raman Spectra: Inorganic and Coordination compounds ; K. Nakamoto; Wiley.
11. NMR, NQR and Mossbauer Spectroscopy in Inorganic Chemistry ; R.V.Parish ;Ellis Horwood.
Course No: CH14305EA  
Title: Industrial Pollution and Green Chemistry (04 Credits)

Max. Marks: 100  
External Exam: 80 Marks.  
Duration: 64 Contact hours  
Internal Assessment: 20 Marks

Unit-I: Industrial Pollution.  
(16 Contact 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  
(16 Contact 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  
(16 Contact hours)

Unit-IV: Green Chemistry-Practice  
(16 Contact hours)
Green Solvents and Reaction conditions: Supracritical fluids, Aqueous reaction conditions, Immobilized Solvents and irritative reaction conditions.
Examples of Green materials, reagents and some specific reactions.

Books Recommended:
7. Green Chemistry- An Introductory Text; IInd Edn.; Mike Lancaster; RSC; 2010.
Course No: CH14306EA
Title: Laboratory Course in Physical Chemistry-II (04 Credits)

Max. Marks: 100
External Exam: 80 Marks.
Duration: 64 Contact hours
Internal Assessment: 20 Marks

A. Conductometry
1. Determination of the composition of a mixture of HCl and CH₃COOH 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 Fe²⁺/Fe³⁺.

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. 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 KMnO₄

Books Recommended:
5. Chemistry Experiments for Instrumental Methods, Sawyer, Heineman, Beebe, Wiley, 1984
Course No: CH14307EO
Title: Philosophy of Science (04 Credits)

Max. Marks: 100
Duration: 64 Contact hours
External Exam: 80 Marks.
Internal Assessment: 20 Marks

Unit-1: Representation. (16 contact hours)
Laws of nature; Knowledge, Sources of knowledge, The rationalists, The empiricists, The Mathematical knowledge, Synthetic Knowledge, Science as knowledge source, Religion and science The Method of science, Induction versus deduction, Representation and reason, minimalism about laws, Laws and counter-factuals, Probabilistic laws, Basic and derived laws, Laws, Regularities and Induction, Necessitation,

Explanation: Kinds of explanation
Natural Kinds; Kinds and classification, Natural kinds and explanatory role.
Realism; Realism and its critics, Instrumentalism, Constructive empiricism, Laws and anti-realism, Anti-realism and inference, Anti-realism and structure of science.

Unit-2: Reason (16 contact hours)
Inductive Scepticism; Theory and observation, Dissolving the problem of Induction, Probability and scientific inference, Kinds of Probability, Classical statistical reasoning.

Inductive Knowledge; Reliabilist epistemology, reasoning with induction, Innate epistemic capacities and reasoning about induction, Internalism and justification.

Method and Progress; Methodology of scientific research programmes, Clinical trials and the scientific method, The content of discovery and the context of justification, Science without the scientific method, Method and the development of sciences, Paradigms and Progress.

Unit-3: Classical Determinism and Probabilistic world (16 contact hours)
The Classical Mechanics; Mechanistic determinism, General principles; Equations of motion, Action at a distance, Electric and magnetic forces, The Failures of the classical mechanics; Atomic structure, The problem of radiation, Motion in time and space.

The birth of modern science; The photo-electric effect, The atomicity of radiation, Particle-wave duality, waves of probability, Uncertainty principle, subject versus object, The fundamental laws of radioactivity; The new Quantum theory; wave mechanics, Diracs Quantum mechanics, The new philosophical principles; the probabilistic reasoning.

Unit-4: The Dawn of Modern Thinking (16 contact hours)
The arrow of Time: From Descarts to quantum theory. The relation of quantum theory to other natural sciences. Language and reality in modern science. The role of modern science in the present development of human thinking.
Books Recommended:
1. Philosophy of science, Alexander Bird, McGill-Queen's University Press.
2. Physics and Philosophy, W. Heisenberg, Harper Perennial Modern Classics
4. Reconstruction of religious thought in Islam, Muhammad Iqbal, Adam Publishers & Dodo Press
6. The philosophy of science, David Papineaus, Oxford University Press.
7. Reality and Representation, David Papineaus, Blackwell Publication.