# 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.

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: (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 $A_2$, 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. (16 Contact hours)**

**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. (16 Contact hours)

**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. $5^{th}$ 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, $2^{nd}$ Ed., J.Coxon, and B.Halton ($2^{nd}$ Ed. Cambridge University press-1987).
7. Fundamentals of photochemistry, Rohtagi & Mukherjee (Wiley Eastern-1992).

# Course No: CH14302CR

**Title: Physical Chemistry. (04 Credits)**

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

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

General theory of angular momentum. Eigen functions and Eigen values of angular momentum operators. Ladder operators. Spin angular momentum, antisymmetry and Pauli's principle. Wave functions of poly-electron atoms, Slater determinant. Atomic term symbols, term separation of pn and dn configurations, spin-orbit coupling, Zeeman splitting.

### 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.

## Unit-II: Quantum Chemistry-II (16 Contact hours)

### Chemical Bonding

LCAO-MO approximation, $H_2^+$ molecular ion, brief introduction to $H_2$. Molecular term symbols. Valence bond treatment of $H_2$, comparison of MO and VB methods in the light of $H_2$ molecule. Hybridization of orbitals (sp, sp2 &sp3 ).

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

Alternant hydrocarbons, Naphthalene, heteroatomic conjugated systems. Limitations of Huckel theory. Parisar-Parr-Pople method, Extended Huckel Method.

## 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.

**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) (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 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. Molecular Quantum Mechanics - P. W. Atkins and R. S. Friedmann, Oxford, 1997.
6. Coulson's Valence, R. Mcweeny, ELBS.
7. Molecular Thermodynamics of Electrolyte Solutions, Lioyd L Lee, World Scientific, 2008.
8. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
9. Modern Electrochemistry 1, 2A, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
10. Electrochemical methods, Fundamentals and Methods, A.J. Bard, L.R. Faulkner, Wiley, 1980.
11. Physical Electrochemistry- Fundamentals, Techniques and Applications, Eliezer Gileadi, Wiley-VCH 2011.
12. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.

# Course No: CH14303CR
# Title: Laboratory Course in Physical Chemistry-I (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 be 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 $KNO_3$.

## C. 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.
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:***


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

# Course No: CH14304EA

## Title: Selected Topics in Chemistry. (04 Credits)

***Max. Marks:*** *100* ***Duration:*** *64 Contact hours*
***External Exam:*** *80 Marks.* ***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 $\mu_{eff}$ 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.

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-III: Applicaions 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).

Introduction to Raman Spectroscopy. Application of Raman spectroscopy in the study of vibrational modes of Metallo-proteins.

**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. 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. Electronic Spectra of Transition Metal Complexes - D. Sutton (McGraw-Hill, 1968)
6. Elements of Magnetochemistry - R. L. Dutta, A. Syamal (Affiliated East -West, 1993).
7. Physical Methods for Chemistry; 2nd edn., R.S.Drago ; Saunders ; 1992.
8. Structural Methods in Inorganic Chemistry; 2nd edn. E. A. V. Ebsworth & D.W.H. Rankin; ELBS; 1991.
9. Spectroscopy in Inorganic Chemistry; Vols I& II; Rao, Ferraro; Academic;1970.
10. Infrared and Raman Spectra: Inorganic and Coordination compounds ; K. Nakamoto; Wiley.
11. NMR, NQR and Mossbauer Spectrascopy in Inorganic Chemistry ; R.V.Parish ;Ellis Horwood.

# Course No: CH14305EA
# Title: Industrial Pollution and Green Chemistry (04 Credits)

***Max. Marks:*** *100* ***Duration:*** *64 Contact hours*
***External Exam:*** *80 Marks.* ***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)**

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 (16 Contact 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: CH14306EA
# Title: Laboratory Course in Physical Chemistry-II (04 Credits)

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

## 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. 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 $KMnO_4$

***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

# 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 **, S**ources 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
3. Physics and Philosophy, Sir James Jeans,Cambridge University Press
4. Reconstruction of religious thought in Islam, Muhammad Iqbal, Adam Publishers& Dodo Press
5. Philosophy of natural science, Carl G. Hempel**,** Pearson.
6. The philosophy of science, David Papineaus, Oxford University Press.
7. Reality and Representation, David Papineaus, Blackwell Publication.
8. Belief, truth and knowledge, D.M. Armstrong, Cambridge University Press.
9. Modern epistemology, Nicholas Everitt and Alec Fisher, McGraw-Hill Higher Education.
10. The structure of scientific revolution, Thomas S. Kuhn, The University of Chicago Press.