### Ph.D Courses

<table>
<thead>
<tr>
<th>Course Code</th>
<th>Course Title</th>
<th>Credits</th>
<th>Semester</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phy.Chem:811</td>
<td>Surface Chemistry</td>
<td>3.0</td>
<td>13</td>
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<tr>
<td>Phy.Chem:812</td>
<td>Electrodics</td>
<td>3.0</td>
<td>14</td>
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<td>Phy.Chem:813</td>
<td>Thermochemistry and Thermochemical Energetics</td>
<td>3.0</td>
<td>15</td>
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<td>Phy.Chem:814</td>
<td>Heterogeneous Catalysis: II-Applications</td>
<td>3.0</td>
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<tr>
<td>Phy.Chem:815</td>
<td>Ion Exchange</td>
<td>3.0</td>
<td>17</td>
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<tr>
<td>Phy.Chem:816</td>
<td>Radiation Chemistry</td>
<td>3.0</td>
<td>18</td>
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<tr>
<td>Phy.Chem:817</td>
<td>Aquatic Chemistry</td>
<td>3.0</td>
<td>19</td>
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<tr>
<td>Phy.Chem:818</td>
<td>Modern Chromatographic Techniques</td>
<td>3.0</td>
<td>20</td>
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<tr>
<td>Phy.Chem:819</td>
<td>Tribology</td>
<td>3.0</td>
<td>21</td>
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<tr>
<td>Phy.Chem:820</td>
<td>Photochemistry</td>
<td>3.0</td>
<td>22</td>
</tr>
<tr>
<td>Phy.Chem:821</td>
<td>Gas phase Uni-molecular Reactions</td>
<td>3.0</td>
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<tr>
<td>Phy.Chem:822</td>
<td>Mass Spectrometry</td>
<td>3.0</td>
<td>24</td>
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<tr>
<td>Phy.Chem:823</td>
<td>Modern Gas Kinetics</td>
<td>3.0</td>
<td>25</td>
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<tr>
<td>Phy.Chem:825</td>
<td>Special topics in Physical Chemistry</td>
<td>1.0</td>
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<tr>
<td>Phy.Chem:826</td>
<td>Term paper</td>
<td>1.0</td>
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<tr>
<td>Phy.Chem:827</td>
<td>Seminar</td>
<td>1.0</td>
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</tbody>
</table>
1. **Introduction**  
The behavior of solid/gas, solid/liquid, liquid/gas and Liquid/liquid interfaces/Adsorption interfacial, tension, applications of surface Chemistry.

2. **Solid/Gas Interface**  

3. **Solid/Liquid Interface**  
Contact angles and wetting , wetting agents, Detergency. Ore Flotation, Adsorption from solution, Composite isotherms and their interpretation.

4. **Liquid/Gas & Liquid/Liquid Interfaces**  
Adsorption and orientation at interfaces, Surfactants Gibbs adsorption equation and its applications Micells.Mono-molecular films.

5. **Charged Interfaces**  
The Electrical double layer, HelmHotz, Chapman and Stern Treatment of EDL. The surface charged chemistry of oxide / water interfaces. Theory of double layer of adsorption of organic compounds.

### Recommended Books

<table>
<thead>
<tr>
<th></th>
<th>Author(s)</th>
<th>Title</th>
<th>Publisher</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>M. J. Cock</td>
<td>Chemistry of Interfaces</td>
<td></td>
</tr>
<tr>
<td></td>
<td>G. D. Parfitt</td>
<td></td>
<td></td>
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<tr>
<td>2</td>
<td>J. Oscik</td>
<td>Adsorption</td>
<td>E. Harward, 1982</td>
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<td></td>
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<tr>
<td>4</td>
<td>A.W. Adamson</td>
<td>Physical Chemistry of Surfaces</td>
<td></td>
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<tr>
<td></td>
<td>A. Gast</td>
<td></td>
<td>J. Wiley, 1999</td>
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<tr>
<td></td>
<td>W. Stuman</td>
<td>Chemistry of the Solid-water Interface</td>
<td></td>
</tr>
<tr>
<td></td>
<td>B. Sulzlarger</td>
<td></td>
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<tr>
<td>6</td>
<td>Heimerz*</td>
<td>Principles of Colloids and Surface chemistry</td>
<td>Marcel Dekker, 1997.</td>
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<tr>
<td></td>
<td>R. Gopalan</td>
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</tbody>
</table>
1 **Voltametry:**
Current voltage curve, Reversible and irreversible electrode processes, Factors contributing voltage, Different kinds of overvoltages, Hydrogen and oxygen overvoltage, Butler Volmer equation for simple electron transfer reactions, Transfer coefficient exchange current density, Rate constants, Tafel equation

2 **Electrical Double Layer:**
Theory of electrical double layer, Capacity of double layer and its determination, electrocapilirity,

3 **Polarography:**
Principles and applications, Limitation of conventional polarography, applications of polarographic measurements, Different types of polarographic waves and their characteristics.

4 **Modern Electro Analytical Techniques:**
AC polarography, Square wave polarography, RF polarography, Normal and differential pulse polarography.

5 **Corrosion:**
Corrosion and passivation, prevention of corrosion

6 **Fuel Cells:**
Principles, Applications

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**Recommended Books**

1 **J. O. Bockris, A. K. N. Reddy**
   Modern Electrochemistry, Plenum, New York, 1970

2 **C. M. A. Brett and A, M, O, Brett**

3 **F, Scholz (Ed.)**
Introduction:
Specification of chemical processes and thermodynamic properties, thermo-chemical investigations: calorimetric part and chemical part. Temperature dependence of the heat of reaction, Assignment of temperature to chemical process.

Theoretical Background:
Units of energy, thermo-chemical conversion, heat of a process, heats of formation, heat of solution and dilution, heat of ionization, heat of fusion and of transformation.

Thermochemistry of Bonds:
Energy changes in heats of reaction, definition of bond and bond strengths, chemical bond enthalpy and bond energies. Heat of bond dissociation, dissociation energies, crystal energies.

Experimental Methods:
Thermogravimetry, differential thermal analysis and differential scanning calorimetry, thermochemical, dynamic, mechanical and thermoelectric methods, calorimetry, simultaneous thermal analysis techniques.

Computational Thermochemistry:

Recommended Books

1. P. Haines: Principles of Thermal analysis and Calorimetry
2. F. D. Rossini: Experimental Thermochemistry
   Interscience, 1956.
4. K. K. Irikura and D. J. Frurip: Computational Thermochemistry, Prediction and Estimation of Molecular Thermodynamics
Title: HETEROGENEOUS CATALYSIS: II-Applications

1  **Quantitative Aspects of Catalysis by Metals**  
The reactions that metal catalyze, The Volcano Principle.

2  **Heterogeneous Catalysts: Structure, Preparation and Uses**  
Catalyst for industrial processes: general requirements, Catalytic reactors and physical form of catalysts, Composition and manufacture of industrial catalysts: general considerations, Supported metal catalysts, Unsupported metals for use in liquid media.

3  **Heterogeneous Catalysis in Action**  

**Recommended Readings:**

1  M. Bowker  
Basics and Application of Heterogeneous Catalysis  
Oxford, 1998

2  B.C. Gates  
Catalytic Chemistry  
John Wiley, 1992

3  G.C.Bond  
Heterogeneous Catalysis: Principals and applications,  
Oxford, 1987

4  M. Boudart and G.D. Mariadassou  
Kinetics of Heterogeneous Catalytic Reactions,  
Introduction:
Ion exchange reactions, matrix and functional groups, Capacity, Physical structure, Properties of I.E. resins.

Equilibria:

Kinetics:
Mechanism of I.E. processes, Rate laws of ion exchange and diffusion in porous media.

Column Processes:

Applications:
Purification of gases, Dual temperature separations Hydrometallurgy, Medical applications, catalysis by ion exchangers

Recommended Books

1. F. Heltferich  
   Ion Exchange  
   Denver, N. Y., 1995

2. W. Rleman  
   Ion Exchange in Analytical Chemistry  
   H.F. Walton  
   Pergamon, 1970

3. A.E. Rodri  
   Ion Exchange, Science & Technology  
   MartinusNijhoff, Dordecht, 1986

4. C. E. Harland  
   Ion exchange: Theory and Practical  
   Springer Verlag, NY, 1994

5. D.L. Sparks  
   Environmental Soil Chemistry  
   Academic, 1995
Course No. Phy.Chem: 816
Credit Hours: 3.0
Title: Radiation Chemistry

1 **INTRODUCTION**
   General features of radiation chemistry, comparison of radiation chemistry with photochemistry, development of radiation chemistry.

2 **INTERACTION OF IONIZING RADIATION WITH MATTER**
   Sources of ionizing radiation, natural occurring phenomena, man-made sources, characteristics of x-rays, B-rays and -rays, Interaction of electromagnetic radiation, electrons, neutrons and heavy charged particles with matter.

3 **RADIATION DOSIMETRY**
   Dosimetric terms and units, calorimetry, ionization measurements, dosimetry for charged particles and neutrons, chemical dosimetry, Fricke dosimeter and other chemical dosimeters, plastic dosimetry, film dosimetry, fluorescence dosimetry.

4 **WATER AND AQUEOUS SYSTEMS**
   Radiolysis of liquid water, reactive species produced on radiolysis of water and aqueous solutions, characteristics of hydrated electron, hydrogen atom and hydroxyl radicals, radiation chemistry of some important aqueous systems, ferrous sulphate, ceric sulphate, ferrocynide, halide ions and organic systems.

5 **APPLICATIONS OF RADIATION CHEMISTRY**
   Comparison of radiation chemical processes with conventional processes, industrial chemical synthesis, sterilization of medical products, food irradiation, radiation polymerization, pollution control of water and combustion flue gases.

**RECOMMENDED READINGS**

Course No.  Phy.Chem: 817
Credit Hours: 3.0
Title: Aquatic Chemistry

1 **Introduction**
   Goals of the course, water cycle. Influence of man on natural waters. Biogeochemistry and environmental problems.

2 **Review of Kinetics**
   Rate laws, Mechanisms, Factors affecting rates of reactions. Examples from Aquatic chemistry.

3 **Review of Thermodynamics**
   Basic relationships. Free energy and chemical change, Chemical potentials. External factors affecting equilibrium, Non-ideal behavior.

4 **Acids and Bases**
   Basic relationships. PC-pH diagrams, Buffers and buffer capacity, Acidity and alkalinity, Carbonate system. Changes in solution chemistry with the addition of strong acids or bases.

5 **Coordination chemistry**
   Complex stability, Metal ion hydrolysis, Inorganic and organic complexes in natural and polluted water.

6 **Precipitation and Dissolution**
   Solubility product, Common ion effect, Solubility of salts of weak acids and bases, competitive Effects, Carbonate system, Phosphate system.

7 **Oxidation Reduction Reaction**
   Redox equilibria, Pc-PC diagrams, Iron chemistry including corrosion and acid mine drainage, Chlorine chemistry, Biological Redox reactions, Redox Chemistry of water.

**Recommended Books**

1 W. Stumm    J J. Morgan
   Aquatic Chemistry2nd Edition

2 V. L. Snoeylnk D. Jenkins
   Water Chemistry

3 J. F. Pankow.
   Aquatic chemistry Problems,
   Lewis Publishers
Course No: Phy. Chem./818
Credit Hours: 3.0
Title: Modern Chromatographic Techniques

1. **Fundamental Relationships of Chromatography:**
   Retention time, Flow in porous media, Band Broadening mechanism, Parameters affecting resolution, Peak shape models, Retention index system.

2. **Gas chromatograph:**
   Gas liquid chromatography, Preparation of packed columns, Performance evaluation of packed columns, contribution of interfacial adsorption to retention in gas liquid chromatography, Bonded Liquid phases, Porous polymer beads, Gas solid chromatography, Micropacked columns, Capillary columns, The mobile phases in gas chromatography. Instrumental requirements for gas chromatography. Detectors in gas chromatography and their applications. Qualitative and Quantitative analysis in gas chromatography.

3. **Liquid Chromatography:**
   Selection of separation methods, column packing for High Performance liquid chromatography (HPLC), column preparation, Column testing and evaluation, Mobile phase selection in HPLC, Liquid solid chromatography, Polar bonded phases, Reversed phase chromatography, Size exclusion chromatography, Ion exchange chromatography, Ion chromatography, Instrumental requirements for HPLC, High pressure pumps, Detectors for HPLC and their applications, Data acquisition and signal processing, Quantitative analysis, High performance thin layer chromatography.

4. **Techniques of preparative scale chromatography:**
   Gas chromatography, Low and medium pressure liquid Chromatography, High pressure liquid chromatography Countercurrent chromatography.

5. **Hyphenated techniques for identification after chromatographic separation.**
   Interfacing a gas chromatograph to mass spectrometer and Fourier transform infrared spectrometer, Interfacing liquid chromatograph to a nuclear magnetic resonance spectrometer, Gas chromatography-optical emission spectroscopy.

**Recommended Books**

1. **Introduction:**
Definition, history and importance of tribology; tribology as a multidisciplinary subject; nanotribology and biotribology.

2. **Tribological materials:**
Ferrous metals and alloys, nonferrous and alloys, ceramics, cermets, plastics, composites, role of materials mismatch in performance of machine.

3. **Engine components:**
Types, construction, operation, and maintenance of bearings, gears, and pistons.

4. **Wear:**
Wear theories; types of wear; wear of metals, ceramics, and polymers; antiwear measures for the machine components during operation.

5. **Friction:**
Fundamental aspect of friction; types and causes of friction; advantages and disadvantages of friction.

6. **Lubricants:**
History of lubricants; mineral oil based lubricants; vegetable oil based lubricants; lubricating greases; solid lubricants; lubricants additives; commercial lubricants; types of lubrication [hydrostatic lubrication, boundary lubrication, extreme pressure lubrication]

7. **Viscosity:**
Role of viscosity in lubricity of lubricating oils, viscosity index, viscosity index improvers, Newton Concentric Cylinder Experiment, flow of lube oils through a slot; flow of lube oil through a capillary; description and working of viscous oil based hydrostatic step bearings.

8. **Tribometers:**
Working principles, construction, and operation of various tribometers, such as Four-ball wear tester, ball-on-cylinder wear tester, pen-on-disc wear tester.

9. **Current trend in tribology research:**
Development of new antiwear additives for lubricating oils and greases; production of environmental friendly lubricants for the industries and automobile; importance of nanoscience and nanotechnology research in tribology; world-wide role of society of automotive engineers [SAE], and American Standard of testing materials lubrication chemists and engineers, nanoparticles as solid antiwear additives, development of light weight composites for making high performance machine components.
### Recommended books

Course No: Phy.Chem. 820
Credit Hours: 3.0
Title: Photochemistry

1. **PHOTOCHEMICAL PROCESSES**


2. **ORGANIC AND INORGANIC PHOTOCHEMICAL REACTIONS**

   Uni and bimolecular reactions, photo oxidation, Reduction and conduction, chemiluminescence, Reduction of salts.

3. **LAB. TECHNIQUES**

   Irradiation, Actinometry, Spectrometry, Flash photolysis

4. **LASERS**

   Principle of Lasers, Working, Types of Lasers

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**RECOMMENDED BOOKS**

1. C.E. Wayne, R. P. Wayne
   Photochemistry, Oxford, 1997

2. N.J. Turo
   Molecular Photochemistry, University Science Books, 1991

3. A. Cox, T.J. Kemp
   Introductory Photochemistry, McGraw-Hill, 1970
Course No: Phy. Chem. 821
Credit Hours: 3.0
Title: Gas Phase Unimolecular Reactions

1. **Introduction and Early Theories**
   General introduction, Experimental study of unimolecular reaction, Potential energy surfaces, Activated complexes and Absolute rate theory.

2. **Basic Theories of Unimolecular Reactions**

3. **Application of RRKM Theory**
   Calculation of activation parameters for the postulated model of unimolecular gas phase reactions, specification of model for the reaction, Use of NIST kinetics database for gas phase unimolecular reactions. Introduction of NIST Chem rate soft ware for RRKM calculations, Application of RRKM to some important classes of compounds related to combustion and environment.

4. **Experimental Techniques for unimolecular Reactions**
   Thermal Activation Techniques (static and single pulse shock tube methods), Chemical Activation, Photo-activation, electric Discharge Methods.

**Recommended Books**

1. KA Holbrook, MJ Pilling, SH Robertson
   Unimolecular Reactions, 2nd edition
   Wiley, 1996

2. T. Baer W. L. Hase
   Unimolecular Reaction Dynamics: theory and Experiments
   Oxford, 1996

3. P. J. Robinson, K. A. Holbrook
   Unimolecular Reactions
   Wiley, 1972
1. **Introduction**

Atoms, molecules, isotopes, early concepts and experiments, the mass scale and isotopic ratio measurements.

2. **Instrumentation**

Ion source, electron impact chemical ionization, field ionization and field des., photoionization and Resonance, Inductively coupled plasma, Laser microscope, Ion bombardment, Californium-252 plasma desorption. Type of spectrophotometers, single magnetic analyzer, the 60,90 and 180 sectors. Electrostatic analyzers, Double focusing spectrometers. Time of flight tandem systems. GC/MS, Jet separators.

3. **The principles and Methods of Mass Spectrometry**

i. Positive ion production, resolving power, sample introduction, Mass spectra of organic compounds, Qualitative analysis, The measurement of ionization potentials and bond strengths.

ii. Types of ions in mass spectra of organic compounds. Parent or molecular ions, fragment ions, meta stable ions, rearrangement ions, multiple charge ions, ions formed in ion molecule reactions.

iii. Examples of mass spectra of hydrocarbons, oxygen, nitrogen, sulfur, phosphorus, and halogen containing compounds.

4. **Application of Mass Spectrometry to various Disciplines**

Geochemistry, planetary measurements, metals, glasses, ceramics, composites, electronic materials and devices, Air and water monitoring, agriculture and food science, biomedical applications, pharmacology, toxicology and forensic science.

**Recommended Books**

1. Edmond De Hoffmann

2. J.R. Chapman
   Practical Organic Mass Spectrometry

3. R. M. Smith
   Understanding Mass Spectra: A Basic Approach,
   -----------------------------(1998).

4. S. Facchetti
   Mass spectrometry of large molecules,
Title: Modern Gas Kinetics Techniques

1 Thermal Excitation Techniques


2 None Thermal Excitation Techniques (Excitation of Products)


3 Analysis of Experimental Data

Introduction, Normally distributed errors, Linear Regression, Propagation and Combination of Errors, Weighing of Data, None-Linear Least Squares Fits, Matrix Techniques, Goodness of Fit.

Recommended Books


4 I. W. Smith Kinetics and Dynamics of Elementary Gas phase Reactions Butter Worths, 1980
Credit Hours: 3.0
Title: Physical Organic Chemistry

Part-I

BASIC CONCEPTS FOR UNDERSTANDING MECHANISM OF REACTIONS


Part-II

SPECIFIC CHEMICAL REACTIONS


RECOMMENDED READINGS

1. N.S. Issacs  Physical Organic Chemistry
2. H. Maskil  The physical basis of organic chemistry
   Oxford, 1986
3. A. Pross  Theoretical and Physical Principles of Organic Reactivity
4. A. Liberates  Theoretical Organic Chemistry
   McMillion, 1968