

Department of Chemistry
School of Basic & Applied Sciences,
Harcourt Butler Technical University, Kanpur
Curriculum for Doctor of Philosophy (Ph.D.)
Courses

In

Chemistry
Course Code (BCY-701/702/703/704)
Applicable from Session 18-19 for new entrants



HBTU Kanpur
Harcourt Butler Technical University
Nawabganj Kanpur-208002

Department of Chemistry
Harcourt Butler Technical University, Kanpur

Course code	BCY-701			
Category	Compulsory			
Course Title	BASIC CONCEPTS IN CHEMISTRY			
Scheme and Credits	L	T	P	Credits
	3	1	0	4
Pre-requisites	Post graduation in Chemistry/Applied Chemistry			

Course Content:

Chemistry

BCY-701

BASIC CONCEPTS IN CHEMISTRY

Pre Ph.D.

Detailed content

1. General Introduction

- Different types of forces- Covalent bonding, ionic bonding, H-bonding, Vander Waals forces
- Theory of chemical bonding and Group theory

(Lectures: 4-5)

2. Physical Chemistry

i) Thermodynamics: Conservation of energy, Review of Enthalpy, Entropy, Free energy with examples involving chemical systems.

ii) Chemical kinetics and Catalysis: Reaction rate theory, Collision and transition state theory, Potential energy surfaces, Catalysis, Enzyme catalysis.

(Lectures: 7-8)

3. Organic Chemistry

i) Delocalized chemical bonding: Aromaticity, Hyperconjugation, Tautomerism (problems using advance chemistry), Acids and Bases (study of advance problems)

ii) Stereochemistry: Optical activity (with special emphasis on allenes and biphenyls); Chirality; Topicity and prostereoisomerism; Conformations of acyclic and cyclic molecules.

iii) Study of reaction intermediates: Carbocations (Bridge-head carbocation), Carbanions, Free-radical, Benzyne, Nitrenes, Carbenes, N-Heterocyclic Carbenes and their applications in substitution, elimination, addition and Rearrangements reaction.

Applications of Pd(0) and Pd(II) complexes in Stille, Suzuki, Sonogashira, Heck, Negishi and Buchwald-Hartwig coupling Reactions. Palladium and Rh-catalyzed C-H activation.

iv) Hydride transfer reagents: Sodium borohydride, sodium cyanoborohydride, lithium aluminium hydride and DIBAL. Application of boranes (diborane, diisoamylborane, 9-BBN and isopinocampheyl) in organic synthesis.

(Lectures: 10-12)

4. Inorganic Chemistry

- i) **Structure of molecules:** VSEPR theory, Bent's rule, Berry Pseudorotation, Molecular orbital treatment for homonuclear, heteronuclear and delocalized molecules.
- ii) **Acids and Bases:** Measures of acid-base strength; Hard and soft acids and bases.
- iii) **Redox reactions:** Standard electrode potentials, Electromotive forces, Electro-chemical series, Use of reduction potentials.
- iv) **Coordination chemistry:** Bonding in coordination compounds, VBT, MOT and CFT, Electronic spectra of complexes, Magnetic properties of complexes.

(Lectures: 9-10)

5. Spectroscopy:

- Basic Principles and Application of UV-VIS, IR, Mass and NMR spectroscopy.

(Lectures: 4-5)

6. Paper, Thin layer and Column chromatograph:

- Principles, instrumentations, modes of development, Adsorbents, stationary phase, mobile phase, Sampling and application, R_f values, quantitative analysis and applications.

(Lectures: 6-7)

Reference Books:

1. Peter Atkins and de Paula, Physical Chemistry, 7th edition, Oxford University Press Inc., New York.
2. J. E. Huheey, E. A. Keiter; R. L. Keiter, Inorganic Chemistry- Principles of Structure and Reactivity, 4th edition, Pearson's education.
3. J. March, Advanced Organic Chemistry, 5th edition, John Wiley and Sons.
4. F. Albert Cotton, Chemical Applications of Group Theory, 3rd edition, John Wiley and Sons.
5. Instrumental Methods of Analysis, Willard, Merit and Dean.
6. Text book of Quantitative Inorganic Analysis, A. I. Vogel.
7. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman and G. S. Kriz.

Evaluation Scheme

Pre Ph.D. Courses SEMESTER I/II

Course Code	Subject	Credit	CT	AT	TA	Theory Sessional	Semester Final Exam	Grand Total
BCY- 701	Chemistry	4 [3-1-0]	30	10(5T+5P)	10(5T+5P)	50	50	100

Department of Chemistry
School of Basic & Applied Sciences,
Harcourt Butler Technical University, Kanpur

Course code	BCY-702			
Category	Compulsory			
Course Title	ANALYTICAL TECHNIQUES FOR CHEMICAL RESEARCH			
Scheme and Credits	L	T	P	Credits
	3	1	0	4
Pre-requisites	Post graduation in Chemistry/Applied Chemistry			

Course Content:
Chemistry

ANALYTICAL TECHNIQUES FOR CHEMICAL RESEARCH
BCY-702
Pre Ph.D.

Detailed content
Module I

Chromatography

1. Classification of different chromatographic methods: Differential migration, chromatographic process, modes of chromatography distribution coefficient.

(Lectures: 6-7)

2. Theory and practice of chromatography: Sampling and application, capacity factor, column efficiency and resolution, application.

(Lectures:4-5)

i) Paper chromatograph: Modes of development, Sampling and application, R_f values, quantitative analysis and applications.

(Lectures:4-5)

ii) Thin layer chromatography:

Adsorbents, stationary phase, mobile phase, plate preparation, Sampling and application, development and detection of spots, R_f values, applications.

(Lectures:4-5)

iii) Column chromatography:

LC/HPLC: Principles, instrumentations, columns, stationary phase, mobile phase, pumps and applications.

(Lectures:4-5)

Module II

Molecular Spectroscopy

1. UV and Visible Spectroscopy:

Introduction and basic principles, Electronic transitions, Beer-Lambert law, effect of solvent on electronic transitions, Ultraviolet bands for different compounds, Fieser-Woodward rules for conjugated dienes and carbonyl compounds.

(Lectures:4-5)

2. Infrared Spectroscopy(IR):

Principle, Instrumentation, Sample Handling, Zero Point Energy, force constant, anharmonicity, Selection rules, Modes of vibrations, Hot Bands, Fundamental Bands, Overtones, Factors influencing the band position and intensities, Characteristic vibrational frequencies of different compounds, effect of Hydrogen Bonding on vibrational frequencies, FTIR.

(Lectures:4-5)

3. Nuclear Magnetic Resonance(NMR):

Introduction, basic principles, mechanics of measurements, chemical shift, band multiplets, spin-spin splitting, shielding and deshielding effect, coupling constant (J), some characteristics of NMR positions, Application in elucidation of molecular structure, Elementary idea of C^{13} NMR. Fluorine NMR and Nuclear Overhauser (NOE) effect

(Lectures:4-5)

4. Mass Spectroscopy:

Introduction, basic principles, instrumentation, fragmentation patterns, nitrogen rule, interpretation of mass spectra and applications (Advance problems).

(Lectures: 3-4)

Module III

Thermal Methods of Analysis: Thermogravimetric analysis, differential thermal analysis and differential scanning calorimetry.

(Lectures:4-5)

Reference Books:

1. Instrumental Analysis, Douglas A. Skoog, F. James Holler & Stanley R. Crouch.
2. Instrumental Methods of Analysis, Willard, Merit and Dean.
3. Handbook of Instrumental Techniques for Analytical Chemistry Ronald A. Hites, Indian University, School of Public and Environmental Affairs and Department of Chemistry.
4. Applications of absorption spectroscopy of organic compounds, John R. Dyer.
5. Instrumental Methods Analysis, B. K. Sharma.
6. Text book of Quantitative Inorganic Analysis, A. I. Vogel.
7. Spectroscopy of Organic Compounds by P.S. Kalsi, Y.R. Sharma, Robert M. Silverstein & Francis X. Webster.
8. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman and G. S. Kriz.

Evaluation Scheme

Pre Ph.D. Courses SEMESTER I/II

Course Code	Subject	Credit	CT	AT	TA	Theory Sessional	Semester Final Exam	Grand Total
BCY- 702	Chemistry	4 [3-1-0]	30	10(5T+5P)	10(5T+5P)	50	50	100

Department of Chemistry
Harcourt Butler Technical University, Kanpur

Course code	BCY-703			
Category				
Course Title	BASIC CONCEPTS OF ANALYTICAL CHEMISTRY			
Scheme and Credits	L	T	P	Credits
	3	1	0	4
Pre-requisites	Post graduation in Chemistry/Applied Chemistry			

Course Content:

Chemistry

BCY-703

BASIC CONCEPTS OF ANALYTICAL CHEMISTRY

Pre Ph.D.

Detailed content:

1. Solution of chemical concentrations:

Mole, molar mass calculations in grams and moles, molar concentrations, percent concentrations, PPM, PPB, volume ratio for dilution procedures, standard solutions, primary and secondary standards.

(Lectures:9-10)

2. Introduction to analytical chemistry:

Role of analytical chemistry, analytical methods, instrumental analysis, laboratory operations, gravimetric techniques.

(Lectures:5-6)

3. Data analysis:

Classification of errors, accuracy and precision, mean and standard deviations, statistical test of data, calibration curve, RMS.

(Lectures:6-7)

4. Conductometry:

Conductivity, types of conductance, variation with dilution, degree of ionisation, solubility and solubility product, ionic product of water, hydrolysis constant, conductometric titration.

(Lectures:5-6)

5. Electrochemistry:

Reversible and irreversible cells, EMF of cell, Nernst equation, types of electrodes, electrode potential and electrochemical series, different thermodynamic parameters, k , ΔH , ΔS , and ΔG , liquid junction potential and salt bridge, potentiometric titration, concentration cell with and without transference.

(Lectures:5-6)

6. Analysis of water:

Hardness of water, various methods to remove hardness, chemical analysis of water, different methods as alkalinity, free chlorine etc

(Lectures:9-10)

Reference Books:

1. Principles of Instrumental Analysis by Douglas and Skoog, Saunder College Publishing Co., New York.
2. Engineering Chemistry by Jain & Jain, Dhanpat Rai Publication Co., New Delhi.
3. Application of Absorption Spectroscopy of Organic Compounds by John R. Dyer, Prentice Hall of India Pvt. Ltd., New Delhi.
4. Spectroscopy of Organic Compounds by P.S. Kalsi, Y.R. Sharma.
5. Text book of Quantitative Inorganic Analysis, A. I. Vogel.
6. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman and G. S. Kriz.

Evaluation Scheme

Pre Ph.D. Courses

SEMESTER I/II

Course Code	Subject	Credit	CT	AT	TA	Theory Sessional	Semester Final Exam	Grand Total
BCY- 703	Chemistry	4 [3-1-0]	30	10(5T+5P)	10(5T+5P)	50	50	100

Department of Chemistry
Harcourt Butler Technical University, Kanpur

Course code	BCY-704			
Category				
Course Title	RECENT ADVANCES IN CHEMISTRY			
Scheme and Credits	L	T	P	Credits
	3	1	0	4
Pre-requisites	Post graduation in Chemistry/Applied Chemistry			

Course Content:

Chemistry
BCY-704

RECENT ADVANCES IN CHEMISTRY

Pre Ph.D.

Detailed content

1. Green Chemistry

i) Basic Principles of Green Chemistry. Designing a Green Synthesis:

Study of environment friendly reagents, catalysts and their application in organic synthesis. Phase transfer catalysis and solid phase synthesis for environment friendly reactions. Versatile ionic liquids as green solvents. Some examples of synthesis involving basic principles of green chemistry having industrial importance

(Lectures:8-10)

2. Nanochemistry:

Introduction, classification of nanoparticles, synthesis, characterization, properties and application of nanomaterials.

(Lectures:7-8)

3. Surface Characterization by Spectroscopy and Microscopy:

i) SEM (Scanning electron microscopy) - Principles of operation, Instrumentation and applications

(Lectures: 4-5)

ii) TEM (Transmission electron Microscopy): Instrumentation, Basics of Diffraction, and Imaging.

(Lectures: 4-5)

iii) ESR (Electron Spin Resonance): Basic Principles and Magnetic Interactions, Instrumentation and Applications

(Lectures: 4-5)

4. Advanced Materials Chemistry:

Structure of solids, symmetry concepts, crystal structure. Preparative methods and characterization of inorganic solids. Crystal defects and non-Conductivity, stoichiometry. Interpretation of phase diagrams, phase transitions. Basics of magnetic, thermal, electrical, optical and mechanical properties of solids.

(Lectures:7-8)

5. Analytical Techniques for Material Characterization:

Diffraction Methods: X-Ray Diffraction, Neutron Diffraction, Electron Diffraction. Thermal Methods: TGA, DTA, DSC, Thermometric Titration. Adsorption/ Desorption Techniques.

(Lectures:7-8)

Reference Books:

1. Instrumental Analysis, Douglas A. Skoog, F. James Holler & Stanley R. Crouch.
2. Instrumental Methods of Analysis, Willard, Merit and Dean.
3. Handbook of Instrumental Techniques for Analytical Chemistry Ronald A. Hites, Indian University, School of Public and Environmental Affairs and Department of Chemistry.
4. Applications of absorption spectroscopy of organic compounds, John R. Dyer.
5. Instrumental Methods Analysis, B. K. Sharma.
6. Text book of Quantitative Inorganic Analysis, A. I. Vogel.
7. Spectroscopy of Organic Compounds by P.S. Kalsi, Y.R. Sharma, Robert M. Silverstein & Francis X. Webster
8. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman and G. S. Kriz.

Evaluation Scheme**Pre Ph.D. Courses
SEMESTER I/II**

Course Code	Subject	Credit	CT	AT	TA	Theory Sessional	Semester Final Exam	Grand Total
BCY-704	Chemistry	4 [3-1-0]	30	10(5T+5P)	10(5T+5P)	50	50	100

Course Outcome:

After studying the course, the student will be able to:

- Interpret UV-Visible and IR-Spectra.
- Describe a reaction rate having various reaction orders.
- Understand different aspects of corrosion (Chemical and electrochemical corrosion, mechanism, factors affecting, protection and practical problems, prevention methods). Thermodynamic overview of electrochemical processes. Reversible and irreversible cells.
- Gain hands-on experience in making different polymers, distinguish between different polymeric structures, classify polymers and analyze the polymerization mechanism. The uses of polymers in different walks of life.
- Knowledge of conductivity polymers, bio-degradable polymers and fiber reinforced plastics.
- Elucidation of the Thermal Stability of different molecules and their Characterization on the basis of their thermal stability and Glass Transition Temperature of Polymers.
- Analytical separation carried out by Chromatography in a multicomponent system. polymeric structures, classify polymers and analyze the polymerization mechanism. The uses of polymers in different walks of life.
- Determine stability of a substance at elevated temperature, identification, purity and decomposition mechanism of polymers.
- Determine the specific heat, heat of reaction, Melting point & boiling point.
- Check the purity of drugs, crystallization and fusion of polymeric materials.
- Produce gases, basic organic chemicals, detergents, insecticides and sugars.
- Understand the concepts and application of green chemistry.

Evaluation Scheme

Pre Ph.D. Courses

SEMESTER I/II

Course Code	Subject	Credit	CT	AT	TA	Theory Sessional	Semester Final Exam	Grand Total
BCY- 701/702/703/704	Chemistry	4 [3-1-0]	30	10(5T+5P)	10(5T+5P)	50	50	100