#### **BHARATHIAR UNIVERSITY, COIMBATORE-641 046**

#### **B. Sc. CHEMISTRY DEGREE COURSE**

### (AFFILIATED COLLEGES – CBCS PATTERN)

#### (For Candidates Admitted During the Academic Year 2012-2013 Batch & Onwards)

NOTE: THE FOLLOWING PAPER CORE V – CHEMISTRY PAPER IV OF B.SC. CHEMISTRY FROM THE ACADEMIC YEAR 2012-13 IS REVISED AND FURNISHED BELOW. THERE IS NO CHANGE IN THE REMAINING PAPERS.

# **CORE V – CHEMISTRY PAPER IV**

Teaching hours: 45 hours per semester (3 hours per week)

#### Subject description

This paper presents the basic aspects of thermodynamics, adsorption, chromatography and computer programming.

#### Goals

To enable the students to understand the laws of thermodynamics, adsorption and the Computer C Programming.

#### **Objectives**

To study the applications of computer programming in chemistry and the importance

of send and thermodynamics, adsorption and chromatography.

#### UNIT I:

Introduction to second law of thermodynamics – Carnot cycle – entropy – Definition – Entropy changes in isothermal transformation –Trouton's rule. Entropy as function of T and V – Entropy as a function of T and P – Changes of entropy with T, Entropy changes in ideal gas – entropy of mixing of ideal gases.

#### UNIT II

General conditions of equilibrium and spontaneity- conditions of equilibrium and spontaneity under constants – definition of A and G – physical significance of – dA and dG.

Temperature and pressure dependence of G – Gibbs – Helmholtz equation. Chemical equilibrium – The concept of chemical potential – chemical potential in a mixture of ideal gases – van't Hoff Isotherm and isochore – Third law of thermodynamics – statement and applications. Exception to third law.

#### UNIT III ADSORPTION AND CATALYSIS

Adsorption – types, differences between chemisorption and physisorption – Adsorption of Gases by solids – Adsorption isotherms – Freundlich, Langmuir isotherms derivations – BET EQUATION (Derivation not required) – Adsorption from solutions – ion exchange adsorption Types and applications – Techniques to determine the adsorped molecules on solid surfaces.

Catalysis – classification – differences between Homogeneous and Heterogeneous catalysis – Acid Base catalysis – Kinetics and Mechanisms – Autocatalysis – Enzyme catalysis Characteristics and mechanism - Michaelis – Menton equation.

# UNIT IV CHROMATOGRAPHY

Chromatographic methods – Partition Adsorption – Basic principles – Differential migration, adsorption phenomenon, nature of adsorbents, choise of solvents and Rf value – Techniques and applications of Paper, Column and TLC – Gas chromatography and HPLC (Basic principles only).

# UNIT V Some important C programs for Chemistry

Programs: To calculate pH of solution and find that it is basic, acidic or neutral. Calculation of pH of a solution using Henderson equation. To compute the order of a reaction. To compute the half-life period of a reaction. To compute the rate constant of a 1<sup>st</sup> order Reaction. To compute the energy of activation of a reaction.

## **REFERENCES:**

1 .Principles of physical chemistry, B.P.Puri, L.R.Sharma and M.S.Phathania, Shobanlal Nagin Chand & Co.

- 2. Physical chemistry G,W.Castelan, Narosa publishers.
- 3. Physical chemistry(voll1) N.B.Singh, ShivasaranDas,A.K.Singh –New Age International Publishers First edition(2009)
- 4. Introduction to Chromatography V.K.Srivatsava and K.K.Srivatsava S.Chand& Company Second edition(1981)
- 5. Computer for chemists By PundirBansal PragatiPrakasam Pubs