Syllabus
M.Sc. (Chemistry) Programme
(SEMESTER – I)

Group Theory – I
Programme Code- (MSCCH -21)
Course Code – (MSCCH -504)

Group Theory, Instrumentation Chemistry & Computer for Chemist

Block I Symmetry and Group Theory in Chemistry:

Unit 1 Symmetry and Group Theory

Symmetry elements and symmetry operations, definitions of group and subgroup and their characteristics, similarity transformation, product of symmetry operations, equivatlent atoms and equivalent symmetry elements, relation between symmetry elements and operation, relation between orders of a finite group and its subgroup. Conjugacy relation and classes of symmetry operations, point symmetry (or group) and its classification, Schonfliess symbols, representation of group by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} etc. groups to be worked out explicity), products of symmetry operations. Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use in spectroscopy.

Unit 2: Matrix

Matrix, Order of group: denoted by 'h', Character table of symmetry operation, Application of group theory in I.R. and Raman Spectroscopy.

Unit 3: X-ray Diffraction Methods

Bragg condition, Miller indices, Laue's method, Bragg's method, Debye- Scherrer method of X-ray structural analysis of crystals. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules. Ramchandran diagram. General Introduction of Electron Diffraction : Scattering intensity vs scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules.

Block II Chromatographyic and Radioanalytical Methods

Unit 4 Chromatographic methods

Principle, instrumentation and applications of gas and liquid chromatography. Principle and application of TLC, paper, column and HPLC. Ion Exchange chromatography: Cationic, anionic exchangers and their applications.

Unit 5 Gas Chromatography

Theory of gas chromatography, parts of gas chromatograph, detectors (TCD, FID, ECD), Van-Deemter equation (no derivation), concept about HEPT- plate theory and rate theory. Applications.

Unit 6 Radio Analytical Methods

Basic principles and types of measuring instrument, isotope dilution techniques.

Block III

Unit 7 Data Analysis

Types of errors, propagation of errors, accuracy and precision, least square analysis, average standard deviation.

Unit 8 History of development of computers Main frames, Mini, Micro and Super Computer systems. General awareness of computer hardware i.e CPU and other peripheral devices.

Unit 9 Introduction to Computers and Computing

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/Q devices, Secondary storage. Computer languages. Operating system with DOS as an example. Introduction to WINDOWS. Data Processing, principles of programming. Algorithms and flowcharts.

Unit 10 Programming in Chemistry

Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data.

Unit 11 Use of Computer Programmes

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot. Further, the students will operate one or two of the packages such as MATLAB, EASYPLOT, DBASE, and Word Processing software such as MS-WORD and CHEMDRAW.