Semester	**4**
Programme	**CHEMISTRY**
Course	**SKILL ENHANCEMENT (PHYSICAL CHEMISTRY 4)**
Paper Code	**S2CH230411P**
Credits	**4 (PRACTICAL: 4)**
Hours/week	**4 (PRACTICAL: 4)**
Category: Core/MDC/SEC/VEC	**SEC**
Theory/Practical/Composite	**PRACTICAL**
Number of Modules	**2**
Syllabus	**Group A: Introduction to Computer Programming** Basic introduction to programming: Universal Computer Digital data Problem setup Programming languages Introduction to Algorithms and flowcharts Introduction to Fortran 77/Fortran 90/C (any one): Datatypes: integer, real, double precision, complex, character, logical Operators: Arithmetic, logical, character, assignment Input/Output statements: read, write, file manipulation Carriage Control: if-then-else-endif, goto, do loop Inbuilt functions Arrays and their manipulation Gnuplot: Use of graphical software for visualizing important mathematical functions and their properties through 2 D and 3 D graphs Mathematica: Algebraic and numerical calculations using symbolic manipulation programs–Use of Mathematica for simple manipulations **Group B: Introduction to Spectroscopy** 1. To establish the Lambert-Beers law in case of ground state CT complexes 2. Absorption and fluorescence of anthracene-identification of vibronic transitions and mirror-image relation 3. Determination of quantum yield of fluorescence of pyrene or anthracene using quinine sulphate as indicator 4. Identification of simple organic molecules using FTIR spectrometer 5. Determination of Iron or Arsenic content of water by atomic absorption spectrometer

Course Overview	Practical: 1. A high level programming language is introduced (fortran 77/90, C). Develop program logic through flowcharts, compile simple programs, usage of dimensioned variables, plotting of functions using gnuplot. 2. Various spectroscopic techniques and instruments (like absorption, fluorescence and FTIR) are introduced.
Course Outcomes	Upon successful completion of this course, students will be able to: **CO1**: Design logical algorithms and flowcharts to solve numerical and chemical problems. **CO2**: Write, compile, and execute programs in Fortran/C to perform algebraic calculations and data manipulation. **CO3**: Utilize Gnuplot and Mathematica to generate and interpret 2D/3D graphical representations of complex scientific functions. **CO4**: Verify the Lambert-Beer's law for ground-state charge-transfer (CT) complexes using UV-Vis absorption spectroscopy. **CO5**: Apply absorption and fluorescence spectroscopy to determine the quantum yield of fluorescence and verify vibronic transitions and mirror-image relations in aromatic systems (anthracene, pyrene). **CO6**: Characterize organic molecules using FTIR spectrometry, and determine trace Iron/Arsenic content in water samples by atomic absorption spectrometry (AAS).
Program Outcomes	**PO1**: Fundamental Knowledge: Demonstrate a comprehensive understanding of core concepts in chemistry, including organic, inorganic, physical, analytical, and biochemistry. **PO2**: Laboratory Skills: Acquire hands-on experience in laboratory techniques and instrumentation, applying safety protocols and proper methodologies to conduct experiments and analyse results. **PO3**: Problem Solving: Develop critical thinking and problem-solving skills by applying chemical principles to real-world scenarios, including the ability to design experiments and interpret data. **PO4**: Research Competency: Engage in independent and collaborative research projects, employing scientific methods to formulate hypotheses, conduct experiments, and communicate findings effectively. **PO5**: Interdisciplinary Applications: Understand the interdisciplinary nature of chemistry, exploring its applications in fields such as medicine, environmental science, materials science, and nanotechnology. **PO6**: Communication Skills: Effectively communicate scientific information, both verbally and in written form, to diverse audiences, demonstrating the ability to present complex ideas clearly and concisely. **PO7**: Ethics and Sustainability: Recognize the ethical implications and responsibilities of scientific research and practice in chemistry, emphasizing the importance of sustainability and environmental stewardship in chemical practices.

CO #	Course Outcome Summary	Bloom's Taxonomy (K-Level)	Mapped POs
CO1	Algorithm & Flowchart Design	**K3 (Apply)**	PO1, PO3
CO2	Programming (Fortran/C)	**K3 (Apply), K6 (Create)**	PO2, PO3
CO3	Data Visualization & Symbolic Math	**K4 (Analyze)**	PO2, PO5
CO4	Beer's Law & CT Complexes	**K3 (Apply), K4 (Analyze)**	PO2, PO3
CO5	Photochemistry & Fluorescence	**K4 (Analyze), K5 (Evaluate)**	PO2, PO3
CO6	Instrumental Analysis (FTIR/AAS)	**K4 (Analyze)**	PO2, PO5, PO7

Reading/Reference Lists	1. The Art of Programming Through Flowcharts & Algorithms: by A. B. Chaudhuri, Firewall Media. 2. Algorithm, Pseudocode and Flowchart: Learn Algorithm in Simple Steps: by J. Rawal, P. Rawal and B. Singh, BelTReady. 3. Computer Programming Logic Using Flowcharts: by J. Farrell, Boyd & Fraser Pub. Co. 4. Fortran 77 and Numerical Methods: by C. Xavier, New Age International (P) Ltd, New Delhi. 5. Computer Programming in Fortran 77: by V. Rajaraman, PHI Learning Pvt. Ltd., New Delhi. 6. Introduction to Fortran 77: by Gunther Lemprecht, Viewweg Teubner Verlag. 7. Professional Pragrammer's guide to Fortran 77: by Clive G. Page, University of Leicester, U.K. 8. Computers in Chemistry: by K. V. Raman, Tata McGraw Hill Publishing Company Ltd., New Delhi. 9. Physical Chemistry on a Microcomputer: by J. H Noggle, Little Brown & Co. 10. Gnuplot in Action Understanding Data with Graphs: by Philipp K. Janert, Manning Publications. 11. Banwell, C. N. Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill. 12. Barrow, G. M., Molecular Spectroscopy, McGraw-Hill. 13. Hollas, J. M., Modern Spectroscopy, Wiley India. 14. McHale, J. L., Molecular Spectroscopy, Pearson Education. 15. Wayne, C. E. & Wayne, R. P., Photochemistry, OUP. 16.. Brown, J. M., Molecular Spectroscopy, OUP.
Evaluation	Practical: 100 CA: 95; Attendance: 5
Paper Structure for Theory Semester Exam	