Semester	**4**
Course	**Skill Enhancement**
Paper Code	S2CH230411P
Paper Title	Physical Chemistry 4
No. of Credits	Practical: 4
Theory / Practical / Composite	Practical
Minimum No. of preparatory hours per week a student has to devote	4
Number of Modules	
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

Learning Outcomes	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.
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	