

CURRICULUM PLAN
Dr. Upasana Issar
For B.Sc. (H) Chemistry, III Year (Semester V)
Odd Semester, 2023-2024

Name of Paper & Code: DSE 1: Applications of Computers in Chemistry

UPC: 32177903

Contents	Allocation of Lectures	Month wise schedule to be followed	Tutorial/Assignments/Presentation etc.
<p>Basic Computer system (in brief):</p> <ul style="list-style-type: none"> • Numeric/String constants and variables. • Operating Systems (DOS, WINDOWS, and Linux) • Software languages: Low level and High Level languages (Machine language, Assembly language; QBASIC, FORTRAN and C++) <p>Programming Language – QBASIC; Commands:</p> <ul style="list-style-type: none"> • INPUT and PRINT Commands • GOTO, If, ELSEIF, THEN and END IF Commands • FOR and NEXT Commands • Library Functions (ABS, ASC, CHR\$, EXP, INT, LOG, RND, SQR, TAB and trigonometric Functions) • DIM, READ, DATA, REM, RESTORE, DEF FNR, GOSUB, RETURN • SCREEN, VIEW, WINDOW, LINE, CIRCLE. LOCATE, PSET Commands. • Simple programs using above mentioned commands. 	26	16 th August 2023 – 30 th September 2023	<ul style="list-style-type: none"> • Problem Solving • Doubt Session
<p>Programming Language – QBASIC; Commands (Continued)</p> <ul style="list-style-type: none"> • Programs related to graphics • Matrix addition and multiplication • Solution of quadratic equation • Computer Software Excel, etc to solve some of the plotting or calculation problems. <p>QBASIC programs for Chemistry problems</p> <ul style="list-style-type: none"> • Plotting van der Waal Isotherms (Simple Problem, available in general text books) and observe 	16	01 st October 2023- 31 st October 2023	<ul style="list-style-type: none"> • Problem Solving • Doubt Session • Assignment Distribution and presentations • University Papers Discussion

<p>whether van der Waal gas equation is valid at temperatures lower than critical temperature where we require to solve a cubic equation and calculation of area under the curves (Complicated Problem, not available in general text books).</p> <p>Numerical methods</p> <ul style="list-style-type: none"> Polynomial equations (formula, iteration and Newton – Raphson methods) Binary bisection and Regula Falsi 			
<p>Numerical methods</p> <ul style="list-style-type: none"> Numerical integration (Trapezoidal rule) Simultaneous equations Statistical analysis. Numerical differential <p>Basic Computer system (Continued)</p> <ul style="list-style-type: none"> Hardware and Software; Input devices, Storage devices, Output devices, Central Processing Unit (Control Unit and Arithmetic Logic Unit) Number system (Binary, Octal and Hexadecimal Operating System); Computer Codes (BCD and ASCII) Software Products (Office, chemsketch, scilab, matlab, hyperchem, etc.) Internet application. 	14	01 st November 2023- 30 th November 2023	<ul style="list-style-type: none"> Problem Solving Doubt Session Presentation University Papers Discussion
<p>Basic idea of Molecular Modelling</p> <ul style="list-style-type: none"> Using software like chemsketch, arguslab and Accelerlys JDraw etc for geometry optimization and potential energy surface (local and global minima) 	04	01 st December 2023 – 13 th December 2023	<ul style="list-style-type: none"> Problem Solving Doubt Session Presentation Assignment Collection University Papers Discussion

DR. UPASANA ISSAR
Assistant Professor, Department of Chemistry
Kalindi College, University of Delhi

