Unique Paper Code	:	32177903
Name of the Paper	:	DSE-3: Applications of Computers in Chemistry
Name of the Course	:	B.Sc. (H) Chemistry
Semester	:	V
Duration	:	3 hours
Maximum Marks	:	75

Instructions for Candidates

- 1. Each question carries equal marks.
- 2. Attempt any *four* questions.

Q1

- (a) Convert the following numbers
 (i) (17.25)₁₀ to binary number
 (ii) (111.01)₂ to decimal number
- (b) Express the following as BASIC expressions (i) $x = n(x_1^2-x_1.x_2)/2(a+b)$ (ii) $V = nRT/(P + an^2/V^2)+nb$
- (c) Distinguish between Interpreter and Compiler.
- (d) Explain the following commands
 (i) DEF FNA(x)
 (ii) DIM A (3, 3)
 (iii) RESTORE
- Write a program in BASIC to calculate the mean and standard deviation for following observations obtained in the determination of the lead content in a soil sample
 0.152 ppm, 0.176 ppm, 0.142 ppm, 0.161 ppm, 0.160 ppm

(2, 3, 4, 4, 5.75)

Q2

- (a) Identify the errors in the following statements:
 - (i) Y = aSinX
 - (ii) LET B+C = 40
- (b) What is the purpose of the following Library functions?
 - (i) ABS (X)
 - (ii) FIX (X)
- (c) Explain the use of **SCREEN**, **VIEW** and **PSET** commands in BASIC language.
- (d) Write the output of the following program

10 DIM A\$(5), A(5) 20 FOR I= 1 TO 5 30 READ A\$(I), A(I) 40 NEXT I 50 FOR I= 5 TO 1 STEP -1 60 PRINT A(I); A\$(I) 70 NEXT I 80 DATA AJAY,17,SANJAY, 22,RANI,23,RAMESH,19, VIBHA, 21 90 END

(e) Write a program in BASIC to find the number of times the letter 'e' occurs in the following sentence: *Chemistry is the scientific discipline involved with elements and compounds.*

(2, 3, 4, 4, 5.75)

Q3

- (a) Explain the following terms
 - (i) Debugging
 - (ii) Syntax error
- (b) Describe the following error messages with examples:
 - (i) DATA out of range
 - (ii) FOR without NEXT
- (c) Indicate the errors in the following program. Write the corrected program.

10 PRINT A 20 INPUT A,B 30 FOR I = 1 TO 10 40 FOR J = I+1 TO 10 45 C= 0: D = 0 50 C = A + I + C 60 D= B + J + D 70 NEXT I 80 NEXT J 90 PRINT C, D 100 END

- (d) Write a program in BASIC to draw three concentric circles with centre (160,100) and radii 20, 30 and 40 respectively.
- (e) Write a program in BASIC to evaluate the following series:

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!}$$

The value should be accurate till 4th place after decimal.

(2, 3, 4, 4, 5.75)

Q4

- (a) Identify the error in the following constants if any and correct them.
 - (i) +732
 - (ii) PERIODIC "TABLE"
- (b) Identify error in following variable name if any and correct them.

(i) VOL%

(ii) 1 Day

- (c) Differentiate between pre-defined and user-defined functions.
- (d) Write a program in BASIC to input a number and print whether it is integer or not.

(e) The concentration of H⁺ in a dilute solution of HCl is given by the expression $[H^+]^2 - [HCl]_0 [H^+] - K_w = 0$ Write a program in BASIC to calculate the pH of 10⁻⁷ M HCl solution at 25^oC. (2, 3, 4, 4, 5.75)

Q5

- (a) What is the difference between GOTO and ON....GOTO statement?
- (b) Write a program in BASIC to Print "CHEMISTRY" in a vertical line using FOR NEXT command.
- (c) What is the output of the following program? SCREEN 1 PSET (40, 40) FOR J = 5 TO 25 STEP 5 CIRCLE (40, 40), J NEXT J END

How would the output change if the same program is written in SCREEN 2? How will you change colour of the circle.

- (d) Write a program in BASIC to read a matrix and print its transpose.
- (e) Explain Binary Bisection method for finding root of a function. Write a program in BASIC to find the root lying between 0 and 1 for the following equation using binary bisection method. $x^4 - x - 10 = 0$

(2, 3, 4, 4, 5.75)

Q6

- (a) Differentiate between Defined Function and Subroutine.
- (b) Under what situation LET, INPUT and READ statements are used? Give examples.
- (c) Write a program to calculate ${}^{n}C_{r}$. Where n=6 and r=0 to 4. Output should be printed in three columns with heading n, r and ${}^{n}C_{r}$.
- (d) Write output from the following statements:

10 A = 3 11 B = 16.9 12 C = 123456789 13 D = 0.00001234 14 E\$ = "Delhi" 15 F = B/A 16 PRINT A, B, C, D, E\$, F 17 PRINT 18 G = B\A 19 PRINT A; B; C; D; E\$; F; G

(e) Write a program in GRAPHICS to select a viewport with diagonally opposite points as (150, 5) and (600,180) and to draw a SQUARE in any graphics mode with a SIDE of 50 pixels.

(2, 3, 4, 4, 5.75)