[This question paper contains 10 printed pages.]

**Sr. No. of Question Paper : 814** **E** **Your Roll No.....**

Unique Paper Code : 217607

Name of the Course : **B.Sc. (Hons.) Chemistry**

Name of the Paper : Computer Applications in Chemistry – [CHHT–618]

Semester : VI

Duration : 3 Hours Maximum Marks : 75

**Instructions for Candidates**

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt any **6** questions in all.
3. Question No. **1** is compulsory.
4. Use of simple calculators is allowed.

1. (a) Explain **any 3** of the following terms :

   (i) Virus

   (ii) Byte

   (iii) Hardware

   (iv) Debugging

   (b) Identify the valid and invalid numeric and string variables giving reasons :

   (i) X$y$

   (ii) 8ABC

   (iii) TUBELIGHT

   (c) Write the BASIC equivalent of the following algebraic equations

   (i) $f = 4\pi\left(\frac{M}{2\pi RT}\right)^{3/2} v^2 e^{-mv^2/2RT}$

*P.T.O.*

(ii) $P = \frac{4Z^3}{a_0^3} r^2 e^{-2r/a_0}$

(iii) $\lambda = \frac{h}{(2meV)^{1/2}}$

(d) Identify the errors in the following BASIC statements

(i) For A$ = B$ to D$

(ii) DIM X$ = 20

(iii) LET B+C = 40

(e) Write the expanded form of the following :

(i) BASIC

(ii) ASCII

(iii) PIXEL (3×5)

2. (a) What will be the output of the following programs ?

(i)
```
LET X = 5
LET Y = 10
PRINT TAB(2) ; "X"; TAB(5); "Y"; TAB(10); "Z"
PRINT TAB(2) ; X; TAB(5); Y
FOR I = 1 TO 3
Z = X * I – Y
Z = Z + I
PRINT TAB (10+5*I); Z
NEXT I
END
```

(ii) REM TO FIND THE GRADES

```
FOR I = 1 TO 4
READ X(I)
IF X(I) > = 80 THEN
PRINT X(I),"A"
ELSE IF X(I) > = 60 THEN
PRINT X(I),"B"
ELSE
PRINT X(I),"C"
ENDIF
NEXT I
DATA 50,90,85,70
END
```

(b) Write a program in BASIC to input (using READ ...DATA) and multiply the given matrices X and Y and to print the resultant matrix Z.

$$X = \begin{pmatrix} 43 & 36 \\ 14 & 19 \end{pmatrix} \qquad Y = \begin{pmatrix} 41 & 22 \\ 31 & 53 \end{pmatrix}$$

(c) Write a program in BASIC to calculate sin (X) which is given by the series

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} \qquad (4,4,4)$$

3. (a) When do you get the following error messages ?

(i) Underflow

(ii) Out of DATA

(b) What is the purpose of the following library functions ? Explain each with an example

ABS, SQR, MOD, INT

(c) What are logical and relational operators ? Explain each term giving suitable example.

(d) Write a program in BASIC to calculate pressure (in Pascal) for volume varying from 1 litre to 10 litres in steps of 0.5 litre of a van der Waals gas. The program should print the volume and the corresponding pressure.

$$\left(P+\frac{an^2}{V^2}\right)(V-nb) = nRT \qquad (4,4,4)$$

4. (a) The following data was obtained in the distribution of iodine between $CCl_4$ and water.

| | | | | | |
|---|---|---|---|---|---|
| $C_{org}$ | $8.5 \times 10^{-3}$ | $1.2 \times 10^{-2}$ | $1.75 \times 10^{-2}$ | $2.0 \times 10^{-2}$ | $2.5 \times 10^{-2}$ |
| $C_{aq}$ | $1 \times 10^{-4}$ | $1.5 \times 10^{-4}$ | $2 \times 10^{-4}$ | $2.4 \times 10^{-4}$ | $3 \times 10^{-4}$ |

$$K_d = \frac{C_{org}}{C_{aq}}$$

Write a program in BASIC to fit the above data to a straight line using linear least squares fit.

The program should :

Read and print the above data

Calculate the equation which best fits it using linear least squares fit and Print the value of the distribution coefficient, $K_d$.

Equation of slope is given below :

$$\text{slope} = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$$

(b) (i) Given that the ASCII for the character A is 65 what will be the output of the following program

```
LET X$ = "A"
B = ASC(X$)
C$ = CHR$(B)
D = LEN(X$)
PRINT "THE ASCII FOR";" ";X$;" ";"IS";" ";B
PRINT C$, D
```

(ii) What will be the output of the following ?

```
LET A$ = "1234"
LET B$ = "1000"
LET X$ = A$+B$
LET C = VAL(A$)
LET D = VAL (B$)
LET F = C+D
PRINT C, D
PRINT F
PRINT X$
END
```

(c) Given below is a program in BASIC to find the pH of 0.01 M solution of acetic acid using Newton – Raphson iteration.

Given that

$$K_a = \frac{[H_3O^+]^2}{[HA]-[H_3O^+]}$$

$K_a = 1.85 \times 10^{-5}$, tolerance $= 1 \times 10^{-6}$.

**PROGRAM**

```
REM TO USE NEWTON-RAPHSON METHOD FOR PH
REM X IS HYDRONIUM ION CONC ; KA IS ACID DISSOCIATION CONSTT
REM Y IS THE FUNCTION, Z IS ITS FIRST DERIVATIVE
DEF FNY(X) = _____
DEF FNZ(X) = _____
INPUT "GUESS VALUE OF X";X
REM TO START ITERATION
FOR I = 1 TO 100
        REM CALCULATING FUNCTION Y OF X
        P = FNY(X)
        REM CALCULATING THE FIRST DERIVATIVE
        Q = _____
        X1 = X - (P/Q)
        IF ABS(X1 - X) <= _____ THEN GOTO 100
        _____
NEXT I
PRINT "ITERATION UNSUCCESSFUL": _____
100 PRINT _____ ; X
    PH = _____
    PRINT "PH";PH
200 END
```

(4,4,4)

5. (a) Write the statements in BASIC for the following :

(i) To create a window in graphics in the Screen 1 mode with the diagonally opposite points as (10,10) and (100,100) and to draw a line between (50,50) and (100,50)

(ii) To select a view port 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

(b) What is the purpose of the following library functions ? Explain each with a suitable example :

INT, LOG, SIN

(c) Write a program in BASIC to read and arrange the following names in alphabetical order alongwith their telephone numbers

| | |
|---|---|
| ZEBA | 9810876756 |
| ALKA | 9934587453 |
| PRIYANKA | 9745398540 |
| BABITA | 9888765445 |
| TULIKA | 9756932122 |

(d) What is the output of the following ?

(i)
```
10 CLS
20 SCREEN 2
30 LET Y = 100
40 FOR X = 100 TO 500 STEP 50
50 PSET (X,Y)
60 NEXT X
70 END
```

(ii)
```
10 SCREEN 2
20 LET X = 160: LET Y = 100
30 PSET (X,Y)
40 FOR I = 20 to 70 STEP 10
50 CIRCLE (X,Y), I
60 NEXT I
70 END
```
(2,3,3,4)

6. (a) Given the strings B$ = "FOLLOW LAB SAFETY MEASURES", write a program in BASIC to print the above string in the following manner on the screen using LOCATE command and string library functions.

FOLLOW

LAB

SAFETY

MEASURES

(b) Identify the errors in the following set of statements and rectify them

(i)
```
WINDOW (0,0) TO (100,100)
LINE (20,20 – 80,80),,BOX
PSET (30,35),(35,40)
```

(ii)
```
SCREEN
VIEW (160,100) - (300,180)
CIRCLE 20,(200,150),
LOCATE (20): PRINT "CIRCLE"
```

(c) Explain the function of the following keywords in BASIC with suitable examples

(i) LINE (ii) WINDOW

(iii) VIEW (iv) SCREEN

7. (a) WAP in BASIC to find the increase in enthalpy (ΔH) of $SO_2$ when the temperature changes from 300 to 1100K, using Simpson's rule and the following data

| T/K | 300 | 500 | 700 | 900 | 1100 |
|---|---|---|---|---|---|
| Cp/$JK^{-1}$ $mol^{-1}$ | 39.9 | 46.5 | 50.8 | 53.4 | 54.9 |

Given that

$$\int dH = \int C_p dT$$

What will be the output of the above program ? Give the value of ΔH.

(b) WAP in basic to find the mean and variance of the following data

100,101,102,99,98,97

$$\text{variance} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n}$$

(c) Given below is a program to find the roots of a quadratic equation whose roots are real and unequal. Identify the errors and rewrite the program making corrections.

REM TO FIND ROOTS OF QUADRATIC EQUATION

INPUT A,B,C

```
PRINT CALCULATING D
LET D = B*B – 4 * A
REM CALCULATING ROOTS
LET X1 = – B + SQR (D)/(2 A)
LET X2 = – B + SQR (D)/2* A
PRINT TAB(20); "THE ROOTS ARE X1 AND X2"; X1 AND X2
END                                                    (5,4,3)
```

(1800)