4/12/18 (M)

[This question paper contains 4 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 541 **IC**

Unique Paper Code : 32177903

Name of the Paper : Applications of Computers in Chemistry

Name of the Course : **B.Sc. (H) Chemistry : DSE – 1**

Semester : V

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 **Six** questions in total including question No. **1,** which is compulsory.
3. Attempt all parts of a question together.
4. Use of scientific calculator and logarithmic table is allowed.

1. Attempt any **five** parts. Each question carries 3 marks.

   (a) Write BASIC expressions corresponding to following equations.

i. $p = \frac{RT}{(V-b)} - e^{\frac{a}{b}}$

ii. $k = \frac{1}{t} \ln \frac{a}{(a-x)}$

iii. $C = \sqrt{(3RT/M)}$

(b) Write the full form the following (any three):

(i) BCD

(ii) CPU

(iii) IP

(iv) QBASIC

(c) Differentiate between the following:

(i) High Level Language and Low Level Language

(ii) RAM and ROM

(d) 10100010 is a Binary number. Convert it to Decimal, Octal and Hexadecimal number.

(e) Identify and rectify errors, if any, in the following BASIC constants.

(i) $ 564

(ii) 3.786 E + 40

(iii) 20,349

(f) Name two operating systems. Also list two differences between Software and Hardware.

(g) Differentiate between BIT, BYTE and NIBBLE.

2. Attempt all parts. Each part carries 4 marks.

(a) In a BASIC program where N$ = "APRIL 21, 2018", make use of string library functions LEFT$, RIGHT$ and MID$ to print the output as 21 APRIL 2018.

(b) Write BASIC statements to produce the following

(i) If N has a value less than 40, then transfer control to statement number 30, otherwise execute the next statement.

(ii) Assign 6 to a variable B.

(iii) Assign the value represented by the variable K to the variable N.

(iv) A two-dimensional array to hold 23 items of data.

(c) What is the use of GOSUB and DEFFN

Commands? Explain with suitable examples. (4x3)

3. Attempt all parts. Each part carries 4 marks.

(a) Identify the errors in the following program. Write the correct program.

```
20 CLS: SCREEN   '640*480
25 LOCATE (5, 25): PRINT IDEAL GAS ISOTHERMS
30 VIEW (-100, 100)-(500, 400), , 7
35 WINDOW 0, 30- 0.5, 400
40 FOR T = 200 TO 500 STEP 20
   50 FOR V = 0.05 TO 0.5 STEP 0.0001
      60 P = 0.0821 * T / V
      65 PSET V, P
   70 NEXT T
75 NEXT V
80 END
```

(b) The following program illustrates the use of looping statement

```
INPUT P, Q, M
FOR I = P TO Q STEP M
FACT = FACT * 1
PRINT FACT
NEXT I
END
```

Give three conditions under which this loop will be executed? Also explain what are nested loops?

(c) Explain Regula Falsi Method. Give one example

of its application in chemistry.

4. Attempt all parts. Each part carries 4 marks

(a) Explain briefly about the INPUT and OUTPUT devices in computers.

(b) Identify the valid BASIC variables. Correct the invalid ones.

(i) DEV8

(ii) CHR$

(iii) "ATS"

(iv) MOL-WT

(c) Write output of the following program.

```
CLS
INPUT "ENTER THE NUMBER="; N
PRINT
FOR I = 1 TO 10
T = N * I
PRINT N; "*"; "="; T
NEXT I
END
```

(4x3)

P.T.O.

5. Attempt all parts. Each part carries 4 marks.

(a) Write a program in BASIC to determine the volume of carbon dioxide gas using Newton-Raphson method at 500 K and 100 atm.

Given: a= 3.610 atm dm^6 mol^{-2}; b=0.0429 dm^3/mol; R= 0.0821 1-atm/K/mol.

The equation to be used is

$$PV^3 - (Pb + RT)\,V^2 + a\,(V - b) = 0$$

(b) What is the resolution of Text mode and Graphics mode in BASIC? How will you convert 'screen coordinates' to 'world coordinates'?

(c) Write a program in BASIC using READ----DATA statement to construct and print the transpose of given matrix.

$$X = \begin{pmatrix} 43 & 36 \\ 14 & 19 \end{pmatrix}$$

(4x3)

6. Attempt all parts. Each part carries 4 marks.

(a) Name the three types of BASIC variables. Also differentiate between single and double precision form of real constants.

(b) Write a program in BASIC to calculate the change in entropy (ΔS) of a substance over a given temperature range by the method of integration using the Trapezoidal approximation. Entropy is expressed in terms of the heat capacity at constant pressure as

$$\int_{S_1}^{S_2} dS = \int_{T_1}^{T_2} \frac{C_p}{T}\, dT$$

The heat capacity values at various temperatures for CO are as follows

T/°C	0	10	20	30	40	50	60	70
C_p/J $deg^{-1}mol^{-1}$	28.912	28.902	29.118	29.151	29.184	29.299	29.361	29.392

Use READ----DATA statement to input these values.

(c) What is the purpose of the following commands in BASIC? Explain with example.

(i) DIM

(ii) REM

(iii) RESTORE

(iv) LEN(A$)

(4x3)

P.T.O.

7. Attempt all parts. Each part carries 4 marks.

(a) Explain briefly about the development of computer with respect to its GENERATIONS.

(b) Write a program in BASIC to calculate the mean and the 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.

(c) What would be the output of 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 same program is written in SCREEN 2? How will you change colour of the circle. (4x3)