Unique Paper Code : 32177903

Name of the Paper : DSE-II Applications of Computers in Chemistry

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

Semester : V

Duration : 3 hours

Maximum Marks : 75

Instructions for Candidate

*1. Attempt only **Four** Questions.*
*2. **Question Number 1 is compulsory**. Attempt any three questions out of remaining five questions.*
3. Attempt all parts of a question together.

1. Attempt all parts.

   a. Explain the following terms
      i. Operating System
      ii. Debugging
      iii. ASCII code

   b. Write the full form of the following abbreviations
      i. QBASIC
      ii. PIXEL
      iii. ALU
      iv. BIT

   c. Write the following algebraic expressions in BASIC
      i. $H = antilog(-pH)$
      ii. $p = \frac{nRT}{V-nb} - \frac{an^2}{V^2}$
      iii. $E = \frac{n^2h^2}{8ml^2}$
      iv. $C = Ae^{-kT}$

   d. Identify and correct the incorrect numeric/string variables (IF ANY)?
      i. END
      ii. M 5
      iii. J$6
      iv. 2VOL!
      v. P*5
      vi. PI$
      vii. A1
      viii. XY%

(3,4,4,4)

2.

a. Write a program in BASIC to calculate cosine series for *x*=-1 till the contribution is less than 0.0001

Given: $\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots . \frac{x^n}{n!}$

b. Write a program in BASIC to read, print and carry out the transpose of following matrix

$$\begin{vmatrix} 3 & 4 & 5 \\ 6 & 7 & 8 \\ 1 & 7 & 9 \end{vmatrix}$$

Note that the printing is to be done along with vertical line whose ASCII value in decimal is 179.

(10,10)

3.

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
40 FOR T=200 TO 500 STEP 20
50 FOR V= 0.05 TO 0.5 STEP .0001
60 P=0.0821 *T/V
65 PSET V,P
70 NEXT T
80  END
```

b. Identify which of the following statements, if any are written incorrectlyand write their correct form

i. ON N$ GOTO 10, 20, 30
ii. IF X^2 < 0 THEN 20
iii. FOR I = 10 TO 0 STEP 2
iv. IF X < A+B THEN 55 ELSE 72
v. FOR K$= 1 TO L STEP2
vi. DEF FN(X)= X^4 – Z^3

c. Write a program in BASIC to assign “CHEMICAL THERMODYNAMICS”to string variable A$, extracting required string constants from A$ using onlystring functions/commands print “THERMODYNAMICS CHEMICAL” (Note-None other string constants to be used).

(6,6,8)

4.

a. Convert the following

i. $(422.125)_{10}$ to binary.
ii. $(11101.1101)_2$ to decimal.

b. What is the difference between computer screen coordinates and world coordinates? Give the syntax for changing screen coordinates to world coordinates.

c. Write a program to find the slope (m) and intercept (c) of the straight-line equation Y = mX + c for a set of discrete X, Y data points. Total number ofdata points are N in number. Provide the data using INPUT statement. Use the following expressions.

slope= $\frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - \sum x_i^{\,2}}$ $and\ intercept = \frac{\sum y_i \sum x_i^2 - \sum x_i \sum x_i y_i}{n\sum x_i^2 - \sum x_i^{\,2}}$

d. Identify the errors in the following Basic Numbers. Also write the correctform for the incorrect one.

i. 7,102
ii. 4.63E – 0.8
iii. + - 4251
iv. 2.6E + 2
v. Rs123
vi. 6.91
vii. -6.8×10^{-5}
viii. 456V3

(4,4,8,4)

5.

a. Differentiate between relational and logical operators.
Let X=1 and Y=2. Determine whether the following relational expressions is true or false

i. 2*X+Y^2 > Y+3
ii. X > Y OR X > 0 AND Y < 0

b. Explain Simpson's 1/3 rule for numerical integration. Write a program to determine the enthalpy asgiven by the expression

$$\Delta H = \int_{T_1}^{T_2} (A + BT + CT^2)dT$$

c. Using sorting, write a program in BASIC to arrange the following student's names in alphabetical order along with their CGPA

Student Name	CGPA
KESHAV	7.5
AMITA	8.8
MEGHA	6.4
DHRUV	8.5
TEENA	7.0

What will be the change required in the program in order to sort the resultin ascending order of CGPA?

(10,5,5)

6.

a. Write a program in BASIC to find the change in enthalpy (ΔH) of SO2 when the temperature changes from 300 K to 1100 K using trapezoidal rule and the following data

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

Given that

$$\int dH = \int_{T_1}^{T_2} C_p dT$$

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

b. Define subroutines. Write a program in BASIC to read, print and calculatethe average values of pressure, volume and temperature using subroutine. Given data

Pressure (atm)	26.95	78.55	70.36	88.31	110.46
volume (dm^3)	0.1	0.3	0.5	0.7	0.9
temperature (K)	273	373	473	573	673

(10,10)