

6. (a) How is the "wrap text" feature used in MS Excel?
- (b) What is the \$ symbol used along with the cell address in Excel?
- (c) What is the difference between single subscripted variable and double subscripted variables?
- (d) When do we get the following error messages in a BASIC program?
- (i) Out of data
- (ii) NEXT without FOR (2,2,2,4)

[This question paper contains 8 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 1496

I

Unique Paper Code : 2173522003

Name of the Paper : Computer-Applications in Chemistry

Name of the Course : B.Sc. (Prog.)

Semester : III / V

Duration : 2 Hours

Maximum Marks : 60

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt any **four** questions out of **six**.
3. Attempt all parts of a question together.
4. Use of Non-programmable scientific calculator is allowed and all program must be written in BASIC programming language.

1. (a) Write the full form of following abbreviation :

- (i) RAM
- (ii) BASIC
- (iii) VIRUS
- (iv) LCD
- (v) ASCII

(b) Write a program to estimate the mean and variance of 10 given numbers :

27, 32, 52, 23, 34, 78, 45, 23, 65, 52

(c) Write the output of the following :

- (i) Print "555"
- (ii) Print $20/2*(5)$
- (iii) Print "CARBON", "HYROGEN", "NITROGEN"
- (iv) Print "CHEM"; "PHY"; "MATH"
- (v) Print TAB(2); "GUESS" (5,5,5)

READ P

LET Q = A+L

LET R = A-L

PRINT A, B, C, X, L, M, N, P, Q, R (5,5,5)

5. (a) Write a program to enter the elements of a matrix using READ....DATA statement and print both the original matrix and its transpose in matrix form.

(b) Write the full form of following abbreviation :

- (i) CNDO
- (ii) INDO
- (iii) AM1
- (iv) HOMO
- (v) PM3

(c) What are the non-empirical quantum mechanical method of calculations? Name and explain them.

(5,5,5)

(b) Fill in the blanks :

- (i) _____ statement is not executed in BASIC.
- (ii) _____ is the smallest unit of memory size.
- (iii) _____ is a set of instructions written for the computer.
- (iv) _____ function gives remainder as the output.
- (v) Cell D4 contains the formula = C1+C2. Formula that will be seen when we paste this into cell E5 _____.

(c) Write the output of the following program :

Data 5, -3, 1.7, 2.2

Read A, B

READ C, X

RESTORE

READ L, M, N

2. (a) Write the purpose of following library function.

- (i) RND(X)
- (ii) INT(X)
- (iii) SIN(X)
- (iv) LOG(X)
- (v) ABS(X)

(b) Identify the errors in the following BASIC statement and correct them :

- (i) P= 6.63-E34
- (ii) "VOLUME" = 22.753
- (iii) For A = 12 TO 3
- (iv) k*2 >=100
- (v) for x = 0 to 10 step -2
.....
For y = 0 to 20 step .5
.....
Next x
Next y

- (c) Write a program to find the pH of 0.01M acetic acid solution using the following equation.

$$K_a = \frac{[H_3O^+]^2}{[HA] - [H_3O^+]} \quad \text{where } K_a = 1.85 \times 10^{-5}$$

(5,5,5)

3. (a) Explain the following terms :-

- (i) Software
- (ii) Compiler
- (iii) High level language
- (iv) Antivirus
- (v) Byte

- (b) Write a BASIC formula that corresponds each of the following algebraic expression :

(i) $\left[\frac{2ab}{c+1} - \frac{r}{7(p+q)} \right]^{\frac{1}{2}}$

(ii) $k = A \exp\left(\frac{-E_a}{RT}\right)$

(iii) $f(c) = 4\pi C^2 \left(\frac{m}{2nkT}\right)^{\frac{3}{2}} \exp\left(-\frac{mc^2}{2kT}\right)$

(iv) $K_a = \frac{x \left(x - \frac{K_w}{x} \right)}{\frac{c}{c^0} - x + \frac{K_w}{x}}$

(v) $x = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$

- (c) Write all the steps to get the table of SIN(θ) and COS(θ) and their curves as a output in EXCEL.
(5,5,5)

4. (a) Explain the function of following syntax command:

- (i) DIM
- (ii) CLS
- (iii) GOSUB
- (iv) END
- (v) INPUT