B. Sc. Chemistry Examination, 2022

(3rd Year, 6th Semester, CBCS, Supplementary)

Chemistry

Paper – DSE/Chem/TH/04/C

Application of Computers in Chemistry

Time : Two hours   Full Marks : 40

UNIT : 6043-P

1. (a) Find the answer of the following relational logical expression

   M**N-M/L.NE.A*B*C

   where M=4, N=3, L=7, A=2.0, B=4.0, C=6.0.

   (b) What is the difference between a FORTRAN expression and a statement.

   (c) The following statements contain errors. Identify those errors.

   i) A + B + C + D
   ii) 7=J*K   1+1+1

2. Write down FORTRAN statements to print the following pattern.

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   ****SPECIAL EXAMINATION****
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3. Explain the following format statement.

   55   Format (5x, E10.5 / f6.2, I2, 3(I5, I4))   1

4. Write a general FORTRAN program for the evaluation of the following series.

   $$Y = 1 + \frac{X^2}{2} + \frac{X^4}{4} + \ldots\ldots\ldots + \frac{X^{16}}{16}$$ 4

5. Answer the following questions.
   (a) Citing suitable examples state the essential features of the computed GO TO statement.

   (b) Write the computational steps in the form of a flow chart for calculating the roots of a quadratic equation.

   (c) Write down the differences between a SUBROUTINE subprogram and a FUNCTION subprogram with an example.   2+2+2

6. (a) Write the binary pattern of 164 in a 8-bit machine. Check if there is any loss of data for such representation.

   (b) Carry out the following conversions

   $(1100.10101)_2$ → Decimal

   $(11.77625)_{10}$ → Binary   2+2

7. Answer *any two* of the following questions.

   (i) Elaborate briefly on the origin of round off error in numerical calculations using computers.

   (ii) Describe the difference between accuracy and precision.

   (iii) Describe one advantage and one disadvantage of Newton's method for numerically solving root of an equation.

                                                                               1.5×2

8. Answer the following questions

   (a) State how many significant digits are there in the following numbers :

        (i) 800320; (ii) 0.0140200; (iii) 5030.02; (iv) 40.00320; (v) 1.0030×10^5

   (b) Round off the results of the following mathematical operations up to appropriate significant digits :

        (i) $(9.836\times10^8)/(2.3\times10^3)$; (ii) $0.00105 \times 12.00 \times 3409.0$; (iii) 3.658+12.1 +7.136

   (c) Derive the expression used in Simpson's one-third rule for numerical integration.

                                                                               2.5+1.5+3

9. Describe briefly *any one* of the following numerical methods.

   (i) Bisection Method for finding roots of an equation;

   (ii) Numerical interpolation method for linear least square fit of a given set of data.

   (iii) Solution of linear simultaneous equations using Gauss-Seidel method.