

[ 4 ]

10. Elaborate on *any one* of the following numerical methods: 6

- i) Numerical integration using Extended Simpson's Rule.
- ii) Numerical solution of linear simultaneous equations using Gauss-Seidel method.

Ex/SC/CHEM/UG/DSE/TH/04/C/2023

**B. SC. CHEMISTRY EXAMINATION, 2023**

( 6th Semester )

**CHEMISTRY (DSE)**

**PAPER: DSE/CHEM/TH/04**

Time : Two Hours

Full Marks : 40

**UNIT : 6043-P**

1. a) Find the answer of the following relational logical expression  
 $.NOT.R.AND..NOT.(IK.LE.BK)$   
where  $BK=2.0$ ,  $IK=4$ ,  $R=.TRUE.$
- b) What is the difference between a FORTRAN expression and a statement?
- c) The following statements contain errors. Identify those errors.
  - i)  $A + B = C**2 + D/E$
  - ii)  $H=6.GT.4.0.AND..NOT.7$  1+1+1
2. Express JCB and BOULT as double and quadruple precision variables, respectively in a single FORTRAN statement. 1
3. Write the format statement to print the following as an output (consider  $\phi$  as a blank character).

[ Turn over

[ 2 ]

Roll No. Marks Obtained

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(A blank line)

27 16.5

(A blank line)

33 17.0

(A blank line)

35 15.5

\*\*\*\*\* 2

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

S = 1 - x^2/2! + x^3/3! - ..... + x^13/13! 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 representation of 0.124 in a 8-bit machine. Check if there is any loss of data for such representation, if so, how much in percentage?

[ 3 ]

b) Carry out the following conversions:

(1100.10101)2 -> Decimal

(11.77625)10 -> Binary 2+2

7. Answer any two of the following questions: 2x2=4

i) State briefly the types of error occurring in a numerical calculation.

ii) Describe the difference between precision and accuracy associated with the numerical computation of a result.

iii) Describe two basic stages for finding roots of an equation.

8. Answer the following questions:

a) State how many significant digits are there in the following numbers : 2 1/2

(i) 705020; (ii) 0.030260; (iii) 2025.00; (iv) 100.01020; (v) 2.30050x10^6

b) Round off the results of the following mathematical operations up to appropriate significant digits : 1 1/2

i) 0.00106 x 16 x 3809 ;

ii) 0.00106 x 16.00 x 3809.0 ;

iii) 5.8413 + 23. + 3.361

9. Obtain the expressions of slope and intercept associated with the linear least square fit algorithm for a given set of data. 6