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

   a) Regula falsi Method for finding roots of an equation.

   b) Numerical solution of 1^{st} order differential integration using 4^{th} order Runge-Kutta method.

   c) Solution of linear simultaneous equations using Gauss-Jordan elimination method. 10

B. Sc. (Chemistry) Examination, 2022

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

Chemistry (DSE)

Application of Computers in Chemistry

Paper – DSE/Chem/Th/04

Time : Two hours Full Marks : 40

UNIT: 6043-P

1. a) Write a FORTRAN statement for the following algebraic expression.

$$\text{Sin } A \text{Cos } B - |g - h| + \sqrt{AB}$$

   b) Write an algebraic expression for the following FORTRAN expression.

   2.3*(x + y + z)**6 + (m*n/2*I)**(2*k)

   c) Evaluate the following logical expression, where A = .TRUE., B = .FALSE., C = .TRUE. .NOT.A.OR.. NOT.B.AND..NOT.C 1+1+1

2. How many data statements are needed by the following Read statement? Explain

   Read (5,105) N, P, Q, D, L, T, Z, S, M

   105 Format (I3/(3E10.3)) 1

3. Write relevant FORTRAN statements for the following.

   a) If x is greater than y then p=11.0, if x is less than y then p=12.0, and if x is equal to y then p=13.0.

b) When P lies between 0.0 and 1.0, set Q=P**2, when P lies between 2.0 and 4.0, set Q=P+Z otherwise Q=Z–P. 1+1

4. Given a 2-dimensional array ITR(3, 3),

8	6	–9
7	3	0
–2	4	1

write a program to do the following.

a) Print the values of the elements row-wise.

b) Sum the values of all the elements.

c) Print the values of all diagonal elements.

d) Calculate the product of all diagonal elements. 4

5. a) Write the binary pattern of 16.429125 in a 16-bit machine. Is there any loss of data for such representation, if so how much?

b) Carry out the following conversions

$(1001.11101)_2 \rightarrow$ Decimal

$(6F5.A8)_{16} \rightarrow$ Binary 2+2

6. Answer the following questions.

a) Discuss the features of block *IF* statement giving suitable examples.

b) Write the steps of computation in the form of a flow chart for calculating the product of even numbers occurring between 1 and 10.

c) Write down a complete general FORTRAN program to compute the factorial of a number. 2+2+2

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

a) Elaborate briefly on the general scheme of an iterative method in a numerical analysis.

b) Describe the difference between percentage relative error and approximate percentage relative error.

c) Describe two basic stages for finding roots of an equation. 1.5×2

8. Answer the following questions :

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

i) 905020 ; ii) 0.0040260 ;

iii) 7025.10 ; iv) 30.01020 ;

v) 1.3040×10^5

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

i) 0.00206 × 18 × 5809 ;

ii) 0.00206 × 18.00 × 5809.0 ;

iii) 5.313+21. +2.36

c) Newton's method of finding roots of an equation converges quadratically – justify. 2.5+1.5+3