

PE-499-CV-19
M.Sc. CHEMISTRY (4th Semester)
Examination, June 2022
COMPUTATION CHEMISTRY

Time : Three Hours]

[Maximum Marks : 80
[Minimum Pass Marks : 29

Note : Answer from both the Sections as directed. The figures in the right-hand margin indicate marks.

Section – A (Very short answer questions)

Q1. Answer the following Question

(10x1)

1. In a FORTRAN program I have set $x=2.0$, $a=2.0$ and $b=4.0$ what is the value of y if $y=a*x+b**2/x$?
2. If a Function is real and continuous in the region from a to b and $F(a)$ and $F(b)$ have opposite signs then there is no real root between a and b .
 - a) True
 - b) False
3. The Jacobi iteration converges, if A is Strictly dominant
 - a) True
 - b) False
4. How many assumptions are there in Jacobi's method?
5. Newton forward interpolation formula can be used in _____.
6. Numerical techniques more commonly involve in _____.
7. The Gauss Jordan Method reduces a original matrix into a _____.
8. Romberg Integration is an extrapolation formula of the Trapezoidal rule for Integration.
 - a) True
 - b) False
9. Which method agrees with Taylor's series solution up to term in h^4 ?
10. How many steps does the fourth – order Runge-Kutta method use.

Q2. Answer The following Question: (Short answer questions)

(5x2).

1. What are the basic datatypes in FORTRAN?
2. Find the root of $x^4-x-10 = 0$ approximately upto 5 iteration using Bisection Method. Let $a = 1.5$ and $b = 2$.
3. Find n if $x_0 = 0.75825$, $x = 0.759$ and $h = 0.00005$.
4. Find the degree of the Polynomial $2X^5 + 2X^3Y^3 + 4Y^4 + 5$.
5. Solve the equations using Gauss Jordan method.

$$x + 2y + 6z = 22$$

$$3x + 4y + z = 26$$

$$6x - y - z = 19$$

Section – B (Long answer questions)

12x5

1. Find the root of the given equation to three decimal place using Bisection Method
 $X^2 - 3$ for $X \in [1, 2]$.

Or

Find by Newton's Method the real root of the equation $3x = \cos x + 1$ correct to four decimal place.

$$3x = \cos x + 1$$

2. Solve equation $2x + 5y = 21$, $x + 2y = 8$ using Gauss Jacobi Method.

Or

Find Solution using Newton's backward difference formula.

X	F(x)
1891	46
1901	66
1911	81
1921	93
931	101

$$X = 1925$$

3. Solve by Taylor series method of the equation

$$\frac{dy}{dx} = \frac{x^2 + xy^2}{e^x}, \quad y(0) = 1$$

For $y(0.1)$, $y(0.2)$, $y(0.3)$

Or

Write a FORTRAN program for Runge - Kutta method.

4. Explain the following
- MOPAC
 - CHARM
 - AMBER

Or

Explain features of GAMES quantum chemical package.

5. Explain how to develop utilities spectra and simulation of program in Physical, Organic, and Inorganic chemistry.

Or

Find the root of the given equation to three decimal place using Bisection method:

$$x \log_{10} x = 1.2$$