

U.G. 6th Semester Examination – 2021

CHEMISTRY

[HONOURS]

Discipline Specific Elective (DSE)

Course code: CHEM-H-DSE-P-3

(Advanced Physical Chemistry Practical)

Answer any two.

2x10=20

1. Describe Newton-Raphson method of root finding? Write a Fortran program to solve $w(x) = x^3 - 8$ using Newton-Raphson method. 4+6=10
2. Describe Trapezoidal rule for numerical integration. Use the Trapezoidal rule to evaluate the integral $\int_a^b y(x)dx$ in which function $y(x) = x\sqrt{(16 - x^2)^3}$ with $a = 0.5$ and $b = 3.5$ for both the assigned increment $h = 1.0$ and 0.5 . Compare the results with the numerical value (191.45) obtained from exact integration of the function from an integration table. Interpret your results. 2+3+3+1=10
3. Which software is suitable for visualization of Ligand-receptor interaction predicted by SWISSDOCK server? Do you know any software to visualize distribution of every amino acid in a protein 3-D structure.

Following table gives the census population of a state for the years 1961 to 2001. Find the rate of growth of the population in the year 2001

Year	1961	1971	1981	1991	2001
Population (Million)	19.96	36.65	58.81	77.21	94.61

2+2+6=10

4. Describe Newton's Forward Interpolation Formula.

Given a cubic polynomial with following data points

x	0	1	2	3
f(x)	5	6	3	8

Find $\frac{dy}{dx}$ and d^2y/dx^2 at $x=0$ using Newton's forward interpolation formula. 4+6=10