

2025

CHEMISTRY — HONOURS

Paper : SEC-3

(Introduction to Numerical Methods in Chemistry)

Full Marks : 75

*The figures in the margin indicate full marks.**Candidates are required to give their answers in their own words as far as practicable.*Answer **question nos. 1, 2, 3, 4** (compulsory) and **any four** questions from the rest (**question nos. 5 to 10**).

1. Answer **any ten** questions : 2×10
- (a) What is the IEEE 754 single precision floating point representation of (i) -0.6251 and (ii) 11.325 ?
 - (b) Express the following decimal number in the binary form : (i) 8.0 and (ii) -12.325 .
 - (c) "Convergence of Newton-Raphson method depends on a good guess value of the root."— Explain.
 - (d) How one can implement least square fitting to the function $y = ae^{-bx}$?
 - (e) Write the equation to calculate the derivative with backward difference method for $f(x) = e^x$ at $x = 0$ with $h = 0.05$.
 - (f) Why Trapezoidal rule is called so?
 - (g) For what order of polynomials does the Simpson's $1/3$ rd rule furnish an exact value of the integral?
 - (h) In second order Runge-Kutta method, how many times you have to evaluate the derivative of each step? Write down the working formula.
 - (i) Write down the expression for the second derivative $\frac{d^2y}{dx^2}$ based on central difference formula $f(x) = y$.
 - (j) What is generally meant by single precision and double precision in computer?
 - (k) What are the Fourier sine and Cosine series?
 - (l) State why least square method is often called 'Regression Analysis'.
2. (a) Deduce Newton-Raphson equation using Taylor series approximation. 5
- Or**
- (b) Obtain first order forward difference formula, backward difference formula and central difference formula using Taylor series approximation. $1\frac{1}{2}+1\frac{1}{2}+2$

Please Turn Over

(4711)

3. (a) Find the coefficient 'a' and 'b' if the equation $y = \frac{1}{ax+b}$ is to be fitted using linear regression to a data set $\{x_i, y_i\}$. 5

Or

- (b) Using Lagrange quadratic polynomial, derive Simpson's $1/3$ rd rule of numerical integration for $\int_a^b f(x)dx$. 5

4. (a) Consider the differential equation $\frac{dy}{dx} = f(x, y)$ with $y(x = x_1) = y_1$. Applying Taylor series method around $x = x_1$, derive the expression for solution $y(x = x_1 + h)$. Then, obtain the Euler's formula from the derived expression. 2½+2½

Or

- (b) For a function $f(x)$ with period 2π , write down the Fourier series and then derive the expressions for the corresponding Fourier coefficients. 2+3

5. (a) Consider the van der Waals equation for the compressibility factor z :

$$z^3 - (1 - b')z^2 + a'z - a'b' = 0$$

with $a' = 0.5$ and $b' = 0.1$. Use Newton-Raphson method to find a real root, starting from $z_0 = 1.0$.

- (b) Discuss the main constraint of fixed-point representation. How that constraint is overcome by floating-point representation?
(c) A table of x vs $f(x)$ is given below. Find the value of $f(x)$ at $x = 4$. 4+3+3

x	1.5	3	6
$f(x)$	-0.25	2	20

6. (a) The Maxwell-Boltzmann speed distribution (unnormalized) is given by

$$f(v) = v^2 e^{-\frac{mv^2}{2K_B T}}$$

with $m = 4.65 \times 10^{-26}$ kg, $T = 300$ K and $K_B = 1.38 \times 10^{-23}$ J/K. Hence, estimate the integral

$$I = \int_0^{1000} f(v) dv$$

using Simpson's rule with '6' subintervals.

- (b) Evaluate the integral $I = \int_0^1 \frac{1}{1+x^2} dx$, using the Trapezoidal rule with '8' subintervals.

(3)

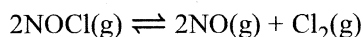
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(c) Certain experimental values of 'x' and 'y' are given below :

x	0	2	5	7
y	-1	5	12	20

If the straight line $Y = a_0 + a_1x$ is fitted to the above data, find the approximate value of a_0 and a_1 .
4+3+3

7. (a) Consider the chemical reaction described by the equation,



at a certain temperature 'T'. If 1 atm of NOCl (g) is introduced into a reaction vessel, the pressures at equilibrium obey the equation,

$$\frac{P_{\text{NO}}^2 P_{\text{Cl}_2}}{P_{\text{NOCl}}^2} = 2.18, \text{ where } k_p = 2.18$$

Solve the equation to obtain P_{Cl_2} at equilibrium using Newton-Raphson method up to four significant figures. Consider the initial guess of P_{Cl_2} as 0.25.

(b) The concentration of a reactant 'A' is monitored over time during a reaction. The following data set is recorded :

time t (s)	0	10	20	30	40	50
Concentration [A] (mol/L)	1	0.82	0.68	0.55	0.45	0.37

Use forward, backward and central difference formulae to numerically estimate the reaction rate at $t = 20\text{s}$.

(c) Use mid point rule to find out the following integral with 5 subintervals :

$$I = \int_0^1 \frac{1}{1+2x} dx \quad 4+3+3$$

8. (a) Find the Fourier coefficients of the periodic function $f(x)$,

$$f(x) = \begin{cases} -K, & -\pi < x < 0 \\ K, & 0 < x < \pi \end{cases}$$

$$\text{and } f(x + 2\pi) = f(x)$$

(b) Determine the linear correlation coefficient 'γ' for the given data set :

x	1	2	3	4
y	0.1	0.4	0.9	1.6

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(4711)

- (c) In a model of nucleation kinetics, the rate of change of concentration $c(t)$ is given by :

$$\frac{dc}{dt} = -\gamma c^2$$

with $\gamma = 0.01 \text{ (mol/L)}^{-1}\text{S}^{-1}$ and $c(0) = 1.0 \text{ mol/L}$.

Use Runge-Kutta fourth order method with $h = 1.0\text{s}$ to find $c(1)$.

4+3+3

9. (a) Estimate the value of ' λ ' and ' c ' by performing least square fit of the equation $PV^\lambda = c$ to the given data :

$P(\text{atm})$	1.13	2.70	5.34	7.86	13.29
$V(\text{L})$	0.82	0.49	0.33	0.25	0.16

- (b) Determine Fourier transform $F(\omega)$ of $f(t) = e^{-t^2}$ by using the definition $F(\omega) = \int_{-\alpha}^{+\alpha} f(t)e^{-i\omega t} dt$.

- (c) For a real gas, the pressure is given by $P(V) = \frac{RT}{V-b} - \frac{a}{V^2}$, where R , a , b and T are constants.

With $T = 350 \text{ K}$, $R = 8.314 \text{ J/(mol K)}$, $a = 0.5 \text{ Pa m}^6/\text{mol}^2$ and $b = 0.03 \text{ m}^3/\text{mol}$, estimate $\frac{dP}{dV}$ at $V = 0.2 \text{ m}^3/\text{mol}$ using a forward difference with $\Delta V = 0.005 \text{ m}^3/\text{mol}$.

4+3+3

10. (a) Use the forward Euler method to solve the initial value problem $y'(x) = xy(x)$, $y(0) = 2$ between $0 \leq x \leq 1$. Consider $h = 0.1$.
- (b) What do you mean by 'residual sum of squares' (SSE) and 'total sum of squares' (SST)? Express 'Coefficient of determination' (r^2) using SSE and SST.
- (c) Determine the Fourier series for $f(x) = x$, $0 \leq x \leq 2\pi$.

4+3+3