Total number of printed pages–16

3 (Sem–5/CBCS) CHE RE 1/RE2/RE3

2021

(Held in 2022)

CHEMISTRY

(Regular Elective)

OPTION – A

Paper : CHE–RE–5016

(Applications of Computers in Chemistry)

Full Marks : 60

Time : Three hours

The figures in the margin indicate full marks for the questions.

1. Answer ***all*** questions : 1×7=7

   (a) What are data processing operations ?

   (b) What is interpolation method ?

   (c) How many bits make a byte ?

   (d) What is variable ?

   (e) What is keyword ?

   (f) What is a string constant ?

   (g) What is iterative method ?

2. Answer ***all*** questions : 2×4=8

   (a) What are library functions ? Give example.

   (b) What is the use of REM statement in a BASIC program ?

   (c) What are structured programming and debugging ?

   (d) What is time-dependent differential equation ? Which one of the following includes a time-dependent differential equation ?

      (i) Chemical reaction (evolution of concentrations with time)

      (ii) Vibrational frequencies.

3. Answer ***any three*** of the following questions 5×3=15

   (a) What do you mean by computer programming ? Write a BASIC program to print positive odd numbers less than 500.

   (b) Describe the different types of operators with examples in BASIC language.

   (c) Write a BASIC program to find the smallest of three input numbers.

(d) Write a BASIC program to find average of n input numbers.

(e) Write a BASIC program to find the numerical value of definite integral.

4. Answer ***any three*** of the following questions : 10×3=30

(a) Explain Newton-Raphson method for finding roots of a real-valued function.

(b) Write a BASIC program to compute the roots of a system of linear equations using Gauss-Seidel method.

(c) The vapor pressure of liquid acetonitrile (CH_3CN) at three temperatures are :

	$T_i(°K)$	P_is $(mm\ Hg)$
1	268.15	20
2	289.05	60
3	300.15	100

Estimate the vapor pressure at 280.15*K* using *(i)* linear interpolation *(ii)* quadratic interpolation.

(d) Explain the functions of following BASIC statements with examples : *(any two)*

(i) DEF

(ii) CALL

(iii) SUB

(e) Write a BASIC program to fit a straight line for the following data relating the enthalpy of methane at 1 *atm* pressure with temperature :

Enthalpy (*Btu/lb*)	630	650	824	851	875	1050	1110	1200
Temperature (°*F*)	−200	−100	0	100	200	300	400	500

(f) What are interpolation and extrapolation ? Explain.