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Gautam Buddha University

Mid Semester Examinations

M.Sc. Applied Mathematics First Semester, (September, 2013)

Course Name: Computational Methods in Chemistry — Maximum Marks: 50
Course Code: CH-501 — Time: 2:00 Hours

Q.1. Attempt ALL parts of the following: $(5 \times 2 = 10)$

(a) There are 365.24 days in a year and exactly 1440 minutes in a day. How many significant digits are in 365.24? How many are in 1440.?

(b) Methane is a compound consisting of a 1 : 4 ratio of carbon and hydrogen atoms. (a) If a sample of methane contains 1565 atoms, how many carbon and hydrogen atoms are present? (b) Can a sample of methane contain a total of 1566 atoms?

(c) Estimate the approximate pressure at 19:64 and 19:66 from the following data:

Time	19:61	19:62	19:63	19:64	19:65	19:66	19:67
Pressure	20	22	26	-	35	-	43

(d) Find $\Delta^6(1-2x)(1-3x^2)(4-7x^3)$ and $\Delta^7(1-2x)(1-3x^2)(4-7x^3)$

(e) Show that $\Delta \equiv E - 1$

Q.2. Attempt ALL parts of the following: $(2 \times 5 = 10)$

(a) Define the following terms and give a suitable example: Commutativity, Associativity, Inverse, Identity, Distributivity.

(b) Define Group. Show that $\mathbb{R}$ (set of real numbers) with addition $(+)$ operation is a group.

Q.3. Attempt ALL parts of the following: $(2 \times 5 = 10)$

(a) We define factorial notation as $x^{(n)} = x(x-1)(x-2)\ldots(x-n\bar{-}1)$. Express $x^2 + 11x + 5$ in factorial notation.

(b) Define Absolute Error, Relative Error and Percentage Error. The diameter and height of a right circular cylinder are measured to be 5 and 8 cm. respectively. If each of these dimensions may be in error by ± 0.1 cm, find the percentage error in volume of the cylinder.

Q.4. Attempt ALL parts of the following: $(2 \times 5 = 10)$

(a) During an experiment we have collected 7 readings, each at one hour distance, 2.3, 4.5, 5.6, 6.7, 7.8,8.9,9.1. Make a difference table and Write the values of $\Delta^2 y_0$ and $\Delta^3 y_1$.

(b) Given $u_0 = 3, u_1 = 12, u_2 = 81, u_3 = 200, u_4 = 100$ and $u_5 = 8$. find the value of $\Delta^5 u_0$

Q.5. Attempt ALL parts of the following: $(2 \times 5 = 10)$

(a) Obtain the first term of the series whose second and subsequent terms are 8,3,0,1,0.

(b) Given $u_0 = 3, u_1 = 12, u_2 = 81, u_3 = 200, u_4 = 100$ and $u_5 = 8$. find the value of $\Delta^5 u_0$