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TERM END EXAMINATIONS (TEE) – December 2021 – January 2022

Programme	: B.Tech.	Semester	: Fall 2021-22
Course Name	: Introduction to Computational Chemistry	Course Code	: CHY1005
Faculty Name	: Dr. Saurav Prasad	Slot / Class No	: B21+B22+B23/0322
Time	: 1½ hours	Max. Marks	: 50

Answer ALL the Questions

Q. No. Question Description Marks

PART - A (30 Marks)

- 1 (a) (i) Newton's law of universal gravitation is represented by 5+5

$$F = \frac{GMm}{r^2}$$

Here F is the gravitational force, M and m are masses, and r is a length. Force has the SI units $\text{kg}\cdot\text{m}/\text{s}^2$. What are the SI units of the proportionality constant G ?

(ii) The radius of a circle is measured to be 11.4 ± 0.5 m. Calculate the area of the circle and the uncertainty associated with it.

OR

- (b) (i) Find the quantum-mechanical operator for p_x^3 . 4+6

(ii) Under what conditions is the function $\exp(-aq^2)$ an eigenfunction of the operator

$$\frac{d^2}{dq^2} - kq^2$$

where k is constant?

(Given: Eigenvalue should not contain terms involving q , so equate the terms involving q to zero.)

- 2 (a) The heats of combustion of C(s, graphite), H₂(g), and CH₄(g) at 298 K and 1 atm are respectively -393.50 kJ/mol, -285.83 kJ/mol, and -890.36 kJ/mol. What is the enthalpy of formation for CH₄? 10

OR

- (b) Show how entropy can be determined by the measurement of the heat capacity as a function of temperature. 10

- 3 (a) (i) Discuss the role of hydrogen bonds in the stability of base pairs in double-helical DNA. 4+6
- (ii) What type(s) of intermolecular forces exist between the following pairs?
- (a) HBr and H₂S
 - (b) I₂ and NO₃⁻
 - (c) NH₃ and C₆H₆

OR

- (b) State the algorithm for performing a Molecular Dynamics (MD) simulation in general and mention the equations involved. Mention the cautions that should be taken while following this algorithm. 10

PART - B (20 Marks)

- 4 In a series of successive measurements in an experiment, the readings of the period of oscillation of a simple pendulum made by Ananya, Hardik, Soumili, Yash, and Sanskriti were found to be 2.43s, 2.96s, 2.22s, 2.81s, and 2.70s, respectively. Calculate (i) the mean value of the period of oscillation (ii) the absolute error in each measurement (iii) the mean absolute error (iv) the relative error, and (v) the percentage error. 10
- 5 Calculate the dipole moment of a water model having following characteristics: $r_{OH} = 0.97 \text{ \AA}$, HOH angle = 104.5° , $q_O = -0.6e$ and $q_H = +0.3e$. What will be the direction of the dipole moment in a water molecule? 10

