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TERM END EXAMINATIONS (TEE) – May 2024

Programme	B.Tech. (All branches)	Semester	Winter 2023-24
Course Name / Course Code	Introduction to Computational Chemistry / CHY1005	Slot	A11+A12+A13
Time	3 hours	Max. Marks	100

Answer ALL the Questions

Q. No.	Question Description	Marks

PART - A – (60 Marks)

1 (a) Perform the following operations and report each answer with the correct number of significant figures: 12

I. 8119×0.0023

II. $42.7 + 0.259$

III. $28.0 / 13.483$

IV. $(5.63 \times 10^2) - (7.4 \times 10^3)$

V. $\frac{(88.5-87.57)}{45.13}$

VI. $\frac{2.8}{1.01} + \frac{62.34}{95} - \frac{84.759}{27}$

OR

(b) Calculate the mean, and the standard deviation for the following frequency distribution: 12

Class interval	1-5	6-10	11-15	16-20	21-25
Frequency	2	3	6	5	4

2 (a) The wavelengths of visible light range from 400 to 750 nm. Calculate the corresponding range of photon energies for visible light. Will the visible light be able to eject an electron from potassium, whose work function is 2.24 eV? 12

OR

(b) The Balmer series is the name given to a series of spectral emission lines of the hydrogen atom that result from electron transitions from higher levels down to the energy level with principal quantum number 2. Calculate the value of wavelengths corresponding to the **first three lines** of the Balmer series in the emission spectrum of atomic hydrogen as per the Bohr atomic model. 12

3 (a) The following sequence of reactions occurs in the commercial production of nitric acid: 12

$4\ NH_3 + 5\ O_2 \rightarrow 4\ NO + 6\ H_2O \quad \Delta H = -907\ kJ$

$2\ NO + O_2 \rightarrow 2\ NO_2 \quad \Delta H = -113\ kJ$

$3\ NO_2 + H_2O \rightarrow 2\ HNO_3 + NO \quad \Delta H = -139\ kJ$

Determine the total enthalpy change for the production of one mol of aqueous nitric acid by this process. The coproducts of the net reaction include H_2O and NO.

OR

(b) The internal energy change when one mol CaCO3 in the form of calcite converts to aragonite is 0.21 kJ. Calculate the difference between the enthalpy change and the change in internal energy when the pressure is 1 bar given that the density of the solids are 2.71 g cm^{-3} and 2.93 g cm^{-3}, respectively. 6

(c) Calculate the amount of heat needed to be supplied to a parcel of air containing 1 mol air molecules to maintain its temperature at 300 K when it expands reversibly and isothermally from 22.0 to 30.0 L as it ascends. 6

4 (a) Define the following and provide an example of each: 12

- Dispersion force
- Dipole-dipole interaction
- Hydrogen bond

Further, on the basis of intermolecular force, explain the differences in the boiling points of n-butane (-1 °C) and chloroethane (12 °C), which have similar molar masses.

OR

(b) Calculate the total number of bonds, bond angles and dihedral angles in **acetic acid dimer** $(CH_3COOH)_2$. Write down the potential energy expression for this molecule as per the molecular mechanics approach. 12

5 (a) Explain the need of periodic boundary conditions (PBC) in molecular dynamics simulations. How do these influence the outcomes of simulations? 12

OR

5 Discuss the importance of using integration algorithms in molecular dynamics simulations. Describe how the Verlet algorithm can be used to compute the next set of positions and velocities. Highlight the advantages and disadvantages of this algorithm. **12**

Part - B – (40 Marks)

6 I. Determine the ΔE between the n = 4 and n = 5 states for an electron trapped within a one-dimensional well of length 3 cm. **8**

II. Plot the wave function and probability density function of an electron trapped in a 1-D box of length 1 Å and having energy 608.4 eV.

7 A student wants to measure g, the acceleration due to gravity, using the equation: **10**

$$g = \frac{2xL}{ht^2}$$

The following values were recorded for each variable:

x: 67.1, 68.2, 78.4, 80.2
L: 100.1, 98.4, 97.9, 102.5
h: 1.10, 1.15, 1.20, 1.00
t: 3.78, 2.95, 3.85, 3.10

Calculate g and its uncertainty based on this data.

8 Arrange each of the following sets of compounds in order of increasing boiling point temperature: **8**

I. HCl, H_2O, SiH_4
II. F_2, Cl_2, Br_2
III. CH_4, C_2H_6, C_3H_8
IV. O_2, NO, N_2
V. LiF, $(H_2O)_2$, $Li^+(aq)$

Provide proper explanation for each.

9 I. The entropy change for the melting of H_2O is 16.2 J/K. During the melting 8 kJ of heat is gained by the system. Comment on the spontaneity of the melting process at −8 °C and at +15 °C. **8**

II. Water is heated on a stove. Does a temperature change from 10°C to 30°C lead to a higher change in entropy than from 45°C to 65°C? Justify using relevant equations.

10 Discuss the significance of time step size in molecular dynamics simulations. How is it determined and what effects can a poorly chosen time step have on the simulations? **6**

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