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TERM END EXAMINATIONS (TEE) – December 2024 - January 2025

Programme	:	B.Tech.	Semester	:	Interim Semester 2024-25
Course Title	:	Introduction to Computational Chemistry	Course Code	:	CHY1005
Date/Session	:	04 Jan 2025/Session I	Slot	:	B22+ B24+ F21
Time	:	3 Hrs.	Max. Marks	:	100

Answer ALL the Questions

Q. No.		Question Description	Marks
		PART A – (60 Marks)	
1	(a)	(i) The speed of light is approximately 3.00×10^{8} m/s and the wavelength of a photon is 6.24×10^{-7} m. Calculate the photon's frequency using $f = c/\lambda$. Calculate the answer with the correct number of significant figures. (ii) A steel rod is measured to be 12.356 cm in length, and its diameter is 0.124 cm. Calculate the volume of the rod assuming it is a perfect cylinder. Report your answer with the correct number of significant figures.	6
	(b)	The force acting on an object of mass m, traveling at velocity V in a circle of radius r is given by $F = mv2/r$ The measurements are recorded as m = (3.5 ±0.1) kg; v = (20 ±1) ms^{-1} and r = (12.5 ±0.5) m. Find the maximum possible (i) relative error and (ii) percentage error in force measurement.	6
		OR	
	(c)	A researcher measures the mass of a sample five times, obtaining the values 2.01g, 2.05g, 1.98g,2.03g, and 2.00 g. Determine the mean mass and the mean absolute error and calculate the relative error and percentage error, assuming the true mass is 2.02 g. Again, Find the standard deviation of the given measurements.	12
2	(a)	An electron is confined in a one-dimensional box of length 1.0 nm, with its motion modeled as a particle in a 1D box. Calculate the energy separations, in joules and electronvolts, between the following levels (a) n = 2 and n = 1, (b) n = 6 and n = 5.	6
	(b)	Identify which of the following functions are eigenfunctions of the operator d/dx: (a) e^{ikx}, (b) cos kx, (c) e^{-ax2}. Give the corresponding eigenvalue where appropriate.	6
		OR	
	(c)	Construct the wave function and probability density plots of the first three electronic states of a particle in a one-dimensional box. Also, write the energy expression of the first, second and third excited states.	12

3 (a) Consider a given reaction,

$$S(g) + O_2(g) \rightarrow SO_2(g)$$

Given at 25°C, change in standard enthalpy and entropy as follows,
i) ΔH_S and ΔS_S are (−376.2 kJ / mol and −233 J /mol)

ii) ΔH_{O2} and ΔS_{O2} are (−212.4 kJ / mol and −142 J / mol)

(iii) ΔH_{SO2} and ΔS_{SO2} are (−976.2 kJ / mol and −153 J / mol). Calculate the Gibbs free energy and equilibrium constant of the reaction.

(b) A sample of 4.50 g of methane occupies 12.7 dm^3 at 310 K. (i) Calculate the work done when the gas expands isothermally against a constant external pressure of 200 Torr until its volume increases by 3.3 dm^3. (ii) Calculate the work that would be done if the same expansion occurred reversibly. 6

OR

(c) Write the relation between Gibbs Free energy with the enthalpy and entropy. Discuss different possibilities of change in enthalpy and entropy leading to the spontaneity of a chemical reaction. 12

4 (a) Classify the following interactions as **dipole-dipole forces**, **London dispersion forces**, or **hydrogen bonding**: 12

(i) The interaction between H_2O molecules and H_2O and Ethanol (C_2H_5OH).

(ii) The interaction between methane (CH_4), ethane (C_2H_6), and propane (C_3H_8) molecules and among them which molecules show higher intermolecular forces.

(iii) The interaction between hydrogen chloride (HCl) molecules.

(iv) Ethanol (C_2H_5OH) and dimethyl ether (CH_3OCH_3) have similar molecular weights. However, ethanol has a much higher boiling point. Explain this observation based on intermolecular forces.

OR

(b) Discuss the Lenard-Jones potential used in molecular dynamics simulations to describe the Van der Waals interaction. For two atoms with ϵ=0.010 eV and σ=0.34 nm, calculate the potential energy U(r) when the separation r=0.4 nm. 12

5 (a) Explain how force fields define the potential energy of a system and mention key components like bond stretching, angle bending, dihedral angles, and non-bonded interactions. 12

OR

(b) In molecular dynamics simulations of a liquid-gel, explain how a Taylor series-based algorithm is used to calculate the next set of positions and velocities. Additionally, discuss the advantages and disadvantages of this approach. 12

PART B – (40 Marks)

6 Perform the operations and report the correct significant figures for the following: 8

(i) 5.2 + 7.589 + 8.52

(ii) (87.323 − 10.02) + 1.21

(iii) 8.453 + 4.3365

(iv) (3.33 × 1.356) / 2.4

7 Calculate the maximum kinetic energy of the ejected photoelectrons when a light of fequency $5.2 \times 10^{14}\ s^{-1}$ falls on the surface of Potassium metal. The threshold wavelength of Potassium is 599 nm. 8

8	Enthalpy and entropy changes of a reaction are 30.5 kJ / mol and 108.8 J / K.mol respectively. Predict the feasibility of the reaction at 27 °C and 500 °C.	8
9	Explain the force field used to calculate bonded and non-bonded interactions. Write the force field equation for C_6H_5COOH and NH_2-CH_2-CH_2-COOH.	8
10	What is molecular Dynamics (MD) simulation? State and explain its application. Write the steps involved in molecular dynamic simulations.	8

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