**Reg. No.:**

**Name :**

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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** | : | **E21+E22+E23/0321** |
| **Time** | : | **1½ hours** | **Max. Marks** | : | **50** |

**Answer ALL the Questions**

| Q. No. | | Question Description | Marks |
|---|---|---|---|
| | | **PART - A ( 30 Marks)** | |
| 1 | (a) | (i) The radius $r$ of a circle inscribed in any triangle whose sides are $a$, $b$, and $c$ is given by $$r = [(s-a)(s-b)(s-c)\ /\ s]^{1/2}$$ where $s$ is an abbreviation for $(a+b+c)/2$. Check this formula for dimensional consistency.<br><br>(ii) Carry out the following arithmetic operations and report in the correct number of significant figures: (a) the sum of the measured values 756, 37.2, 0.83, and 2.5; (b) the product 0.0032 x 356.3; (c) the product 5.620 x π. | 4+6 |
| | | OR | |
| | (b) | A 1.00 g marble is constrained to roll inside a tube of length L = 1.00 cm. The tube is capped at both ends.<br><br>(i) Modelling this as a particle in a one-dimensional box, determine the value of the quantum number *'n'* if the marble is initially given energy of 1.00 mJ.<br><br>(ii) Calculate the excitation energy required to promote the marble to the next available energy state. | 10 |
| 2 | (a) | Determine the enthalpy of the following reaction:<br><br>$3Fe_2O_3(s) + CO(g) \rightarrow 2Fe_3O_4(s) + CO_2(g)$<br><br>given the following data:<br><br>$Fe_2O_3(s) + 3CO(g) \rightarrow 2Fe(s) + 3CO_2(g)$ $\Delta H = -23.44$ kJ<br>$Fe_3O_4 + CO(g) \rightarrow 3FeO(s) + CO_2(g)$ $\Delta H = +21.79$ kJ<br>$Fe(s) + CO_2(g) \rightarrow FeO(s) + CO(g)$ $\Delta H = -10.94$ kJ | 10 |
| | | OR | |

(b) 4.4 kg of carbon dioxide gas, $CO_2$, undergo isothermal expansion at 298 K from a volume of 2 to 5 $m^3$ in three steps of 1 $m^3$. Assuming ideal gas behaviour, what is the total work performed by the gas? 10

3 (a) Identify which of the compounds in each case will have the highest boiling point and justify your choice. 10

i) $CH_4$ and $CH_3Cl$
ii) $C_2H_5OH$ and $CH_3OCH_3$
iii) Methane, Butane, Pentane, and Octane
iv) Hexane, 3-Hexanone, and 3-Hexanol
v) $CH_3CHO$ and $CH_3CN$

OR

(b) 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. 10

## PART - B (20 Marks)

4 Write the Schrodinger equation for hydrogen atom assuming that the charge on the electron is -*e* and that on the nucleus is +*e*. Discuss the various terms involved in this equation. Can this equation be exactly solved? 10

5 Calculate the value of potential energy (in J) of two LJ particles having $\sigma = 0.34$ nm, $\varepsilon =$ 1.65e-21 J and coordinates (in Å) 10

| Particles | x | y | z |
|---|---|---|---|
| 1 | 2 | 2 | 2 |
| 2 | 4 | 4 | 4 |

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