

Reg. No.:

Name :

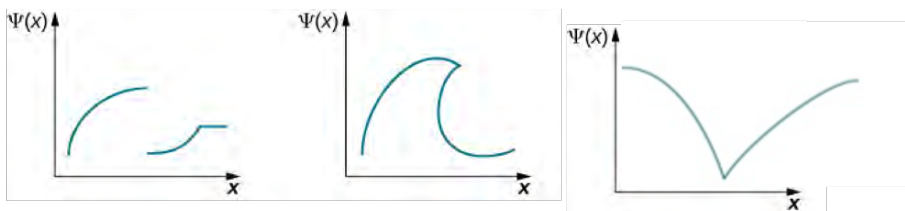


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**Mid-term Examination – November 2021**

Programme	: <b>B.Tech</b>	Semester	: <b>Fall 2021-22</b>
Course	: <b>Introduction to Computational Chemistry</b>	Code	: <b>CHY1005</b>
Faculty	: <b>Dr. Sumit Mittal</b>	Slot/Class No.	: <b>A21+A22+A23/0326</b>
Time	: <b>1½ hours</b>	Max. Marks	: <b>50</b>

**Answer all the Questions**

- | Q. No. | Question Description  | Marks |
|--------|---|-------|
| 1      | Given that $x = (2.4 \pm 0.1)$ s, $y = (1.09 \pm 0.02)$ s, $z = (2.5 \pm 0.3)$ s, calculate the value of $S = x*y + z^2$ and uncertainty associated with it.  | 10    |
| 2      | An empty measuring cylinder is weighed as $12.24 \pm 2$ g. Ramesh transfers $6.4 \pm 1$ mL of HCl solution into the cylinder. Afterwards, the mass of the cylinder increases to $24.020 \pm 2$ g. Calculate the density of the liquid in g/mL. Report the results as per the correct number of significant figures.                   | 10    |
| 3      | Predict whether the following wavefunctions are valid solutions for Schrödinger's equation. Justify your answer.  | 10    |
|        |   |       |
| 4      | "A photon from visible region of light has enough energy to excite an electron from the ground state of hydrogen atom to its fourth excited state." Comment on the correctness of the above sentence. Provide mathematical support.   | 10    |
| 5      | Consider one mole of $H_2O(g)$ which occupies 20 L at 1 atm. Condensation of $H_2O(g)$ at 1 atm releases 30.22 kJ/mol of heat to the surrounding. Given that the density of $H_2O(l)$ at 373 K is 0.925 g/cm <sup>3</sup> , calculate the change in the internal energy for the condensation of one mole of water at 1 atm and 373 K. | 10    |

