VIT®

BHOPAL

www.vitbhopal.ac.in

Mid-Term Examinations – November 2021

Programme	:	**B. Tech.**	Semester	:	**Fall 2021-22**
Course	:	**Introduction to Computational Chemistry**	Code	:	**CHY1005**
Faculty	:	**Dr. Saurav Prasad**	Slot/ Class No.	:	**E21+E22+E23/0321**
Time	:	**1 ½ hours**	Max. Marks	:	**50**

Answer all the Questions

Q.No.	Sub. Sec.	Question Description	Marks
1		Suppose you are told that the acceleration a of a particle moving with uniform speed v in a circle of radius r is proportional to some power of r, say r^n, and some power of v, say v^m. How can you determine the values of n and m?	10
2	(a)	The temperatures of two bodies measured by a thermometer are $t_1 = 25\ ^0C \pm 0.7\ ^0C$ and $t_2 = 52\ ^0C \pm 0.6\ ^0C$. Calculate the temperature difference and the error therein.	5
	(b)	Solve (show intermediate steps too) and report as per the correct number of significant figures: (i) $\frac{2\cdot45+6\cdot89}{4.001} + 4.67$ (ii) $8\cdot61 \times 2\cdot215 - \frac{3.456}{2.54}$	5
3		Laplacian operator $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ in spherical polar coordinates is given by $\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial^2\phi}$. Show that function $\frac{\sin\theta\sin\phi}{r^2}$ is an eigenfunction of the Laplacian operator and find the corresponding eigenvalue.	10
4		The ground-state wavefunction for a particle confined to a one-dimensional box of length L is $\psi = \sqrt{\frac{2}{l}}\sin\left(\frac{\pi x}{l}\right)$. Suppose the box is 10.0 nm long. Calculate the probability that the particle is (a) between x = 4.95 nm and 5.05 nm, (b) in the right half of the box. Use: $\cos(2x) = 1 - 2\sin^2 x$	10
5		How can Gibb's free energy of the system and entropy of the universe be used to determine the spontaneity of a chemical process? Derive the relation between them. A reaction with $\Delta H = +21\ kJ\ mol^{-1}$ and $\Delta S = +41\ J\ K^{-1}\ mol^{-1}$ is non-spontaneous at room temperature. Find the temperature above which the reaction will be spontaneous.	10

⇔⇔⇔