Reg. No.:

Name :

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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.	:	**B21+B22+B23/0322**
Time	:	**1 ½ hours**	Max. Marks	:	**50**

Answer all the Questions

Q.No.	Sub. Sec.	Question Description	Marks
1		Two resistors of resistances $R_1 = 200 \pm 3$ *ohm* and $R_2 = 300 \pm 4$ *ohm* are connected (a) in series, (b) in parallel. Find the equivalent resistance of the (a) series combination, (b) parallel combination. Use for (a) the relation $R = R_1 + R_2$, and for (b) $\frac{1}{R'} = \frac{1}{R_1} + \frac{1}{R_2}$ and $\frac{\Delta R^1}{R'^2} = \frac{\Delta R_1}{R_1^2} + \frac{\Delta R_2}{R_2^2}$.	**10**
2	(b)	A famous relation in physics relates 'moving mass' m to the 'rest mass' m_o of a particle in terms of its speed v and the speed of light, c. Soumili recalls the relation almost correctly but forgets where to put the constant c. She writes : $$m = \frac{m_0}{(1 - v^2)^{1/2}}$$ Guess where to put the missing c with proper reasoning.	**5**
	(b)	State the number of significant figures in the following : (a) 0.007 m^2 (b) 0.2370 g cm^{-3} (c) 6.320 J (d) 6.032 N m^{-2} (e) 0.0006032 m^2	**5**
3		Calculate the percentage change in a given energy level of a particle in a cubic box when the length of the edge of the cube is decreased by 10 percent in each direction.	**10**
4		The normalized wavefunctions for a particle confined to move on a circle are $\psi(\phi) = \left(\frac{1}{2\pi}\right)^{1/2} e^{-im\phi}$, where m = 0, ±1, ±2, ±3, . . . and $0 \le \phi \le 2\pi$. Determine $\langle\phi\rangle$ (expectation value of ϕ). The operator for ϕ is just multiplication by ϕ.	**10**
5	(a)	Can heat flow spontaneously from hot body to cold body? Which law of thermodynamics explains this phenomenon? Explain in detail.	**5**
	(b)	Do all spontaneous reactions lead to an increase in entropy of the system? Justify your answer.	**5**

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