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PG CBCS

M.Sc. Semester-I Examination, 2021

CHEMISTRY

PAPER: CEM 101

(PHYSICAL CHEMISTRY-I)

Full Marks: 40 **Time: 2 Hours**

Answer any <u>FOUR</u> questions: 4X10=40

1. (a) Evaluate the result of the operator (i) $x^2\frac{d^2}{dx^2}$; (ii) $\frac{d^2}{dx^2}x^2$ operating on the function, $x^2 + x + 1$.

   (b) Evaluate the commutator $[\hat{x}^n, \hat{p}_x]$.

   (c) Is the function Ae^{-ax} an eigen function of the operator $\frac{d^2}{dx^2}$? what is the eigen value?

   (d) Which of the following functions meet the requirements for acceptable wave function ψ.

   (i) e^{-ax} (for $-\infty \leq x \leq +\infty$ and a is constant)

   (ii) e^{-x} (for $0 \leq x \leq +\infty$) (2+2) +2+2+2

2. (a) What is the probability of locating the electron confined to a molecule of length l nm between $0 \leq x \leq 0.2$ nm in its lowest energy state?

   (b) Show that the linear momentum operator is Hermition one.

   (c) Normalise the wave function given by $\psi = \sin\frac{n\pi x}{l}$ for a particle moving in a one-dimensional box of length 'l'. (4+3+3)

3. Using Maxwell relations derive thermodynamic equations of State? Why these are called 'thermodynamic equations of state'? (8+2)

4. (a) What is fugacity?

   (b) State third law of thermodynamics?

   (c) Establish the relation between entropy and thermodynamic probability. (3+2+5)

5. (a) Write down the expression for the Boltzmann distribution in terms of energy multiplier β and molecular partition function. Explain the significance of the partition function and state the consequence of the sign of β being negative.

   (b) Obtain the expression for energy in terms of the molecular partition function.

   (1+3+3) +3

6. Explicitly stating the assumptions, deduce the Bose-Einstein distribution equation. What are bosons and fermions? Give one example of each. (6+4)

(P.T.O.)

7. What are the benefits of nanotechnology in electronics? How are gold nanoparticles synthesized? (5+5)
8. What are the benefits of nanotechnology in health and medicine? How are silver nanoparticles synthesized? (5+5)
9. Classify the following molecules with an explanation based on the moment of inertia of the molecule. The following molecules are benzene, water, cyclobutadiene, methane, ammonia, acetylene, chloroform, methylacetylene, boron trichloride, and sulfur hexafluoride. (1×10)
10. (a) Give the expression for vibrational energy of a diatomic molecule taking it as a simple harmonic oscillator. Sketch the vibrational energy levels of such a molecule. Define zero-point energy.

    (b) State the consequence of anharmonicity to a diatomic oscillator.

    (c) The vibrational frequency and anharmonicity constant of a diatomic molecule are 300 cm^{-1} and 0.0025 respectively. Find out the positions of the fundamental and first overtone band. (1+2+2) +2+3

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