Total Pages: 2

PG CBCS

M.Sc. Semester-I Examination, 2020

CHEMISTRY

PAPER: CEM 101

(PHYSICAL CHEMISTRY-I)

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

Answer any four questions: **10X4=40**

1. (a) Find the eigenvalue of the operator $\hat{A} = d^2/d\phi^2$ operating on the wave functions

$$\Phi_m(\phi) = e^{im\phi} \text{ and } \Phi_{-m}(\phi) = e^{-im\phi}$$

Show that any linear combination of the wave functions $\Phi_m(\phi)$ and $\Phi_{-m}(\phi)$ is also an eigenfunction of the operator $\hat{A} = d^2/d\phi^2$.

(b) The wave functions for a particle restricted to lie in a rectangular region of lengths a and b (a particle in a two-dimensional box) are

$$\psi_{n_x n_y}(x,y) = \left(\frac{4}{ab}\right)^{1/2} sin\frac{n_x \pi x}{a}\ sin\frac{n_y \pi y}{b} n_x = 1,2,\ldots \quad 0 \le x \le a$$
$$n_y = 1,2,\ldots \quad 0 \le y \le b$$

Show that these wave functions are normalized. (2+3)+5

2. (a) Evaluate the commutator $[\hat{X}, \hat{P}_x]$, where $\hat{X}$ and $\hat{P}_x$ indicate position and momentum operator respectively.

(b) Show that $\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = 0$ for a particle in a box, for which

$\psi_n(x) = \left(\frac{2}{a}\right)^{1/2} sin\frac{n\pi x}{a}$ $\quad 0 \le x \le a$ (5+5)

3. Define the term Chemical Potential. Derive the Gibbs-Duhem equation and give its applications. (2+6+2)

4. Explain the term fugacity. How is fugacity of a gas determined? 5+5

5.(a) Write, without derivation, 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 in relation to the relative population of the molecules if the sign of β be negative.

(b) Obtain the expression for entropy in term of molecular partition function. (1+3+3) +3

6. Starting from the appropriate expression for thermodynamic probability of distribution, obtain the Bose-Einstein distribution law. What are bosons and fermions? Give one example of each. 6+4
7. State the application of Nanotechnology in electronics. How do you synthesise gold nanoparticles? 5+5
8. State the application of Nanotechnology in health and medicine. How do you synthesise silver nanoparticles? 5+5
9. Classify the following molecules on the basis of their moment of inertia:
   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 simple harmonic oscillator. Sketch the vibrational energy levels of such a molecule. Define zero point energy.
    (b) What type of vibrational spectrum is expected for simple harmonic oscillator in the form of a diatomic molecule?

(1+2+2) +5

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