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PG CBCS
M.SC. SEMESTER-I EXAMINATION, 2022
CHEMISTRY
PAPER: CEM 101
(PHYSICAL CHEMISTRY - I)

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

GROUP – A

1. Answer any FOUR questions from the following questions: **4×2 = 8**

a) What is the orthonormal function? Write down the criteria.

b) Determine the eigen value of Ae^{mx} with respect to $\frac{d^2}{dx^2}$.

c) What do you mean by accessible microstates of a system?

d) What are the conditions for a system of particles to obey Maxwell-Boltzmann statistics?

e) What is a fermion? Give an example.

f) Define morse potential.

g) State the consequence of anharmonicity to a diatomic oscillator.

h) Write applications of rotational spectroscopy.

GROUP - B

2. Answer any FOUR questions from the following questions: **4×4 = 16**

a) Write down the forms of Lx, Ly, and Lz operators starting from r × p vectors.

b) What are the properties of a well-behaved wave function? Check that, the wave function $\psi(x) = A \sin\left({}^{m\pi x}/_{L}\right)$, integration range $0 \leq x \leq L$ is a well-behaved one or it is not. (2+2)

c) What is a stationary state in quantum mechanics? Write the importance of the stationary state of a system. (2+2)

d) Write the Nernst heat theorem. Write the limitations of this theorem. (3+1)

e) Establish the relation between entropy and thermodynamic probability.

f) Define the terms macrostate and microstate.

g) Classify the following molecules with an explanation based on the moment of inertia of the molecule. The following molecules are benzene, water, cyclobutadiene, and methane. (1×4)

h) Obtain the expression for internal energy in terms of the molecular partition function.

P.T.O.

GROUP - C

3. Answer any TWO questions from the following questions: **$2\times8 = 16$**

a) What is the linear operator? What is a Hermitian operator? Write down two important properties of Hermitian operators that have significant roles in quantum mechanics. Prove that the linear momentum operator is a Hermitian operator. (Consider the wave function $\psi(x) = A \operatorname{Sin}\left(m\pi x/L\right)$, integration range $0 \leq x \leq L$). (2+2+2+2)

b) Starting from the appropriate expression for the thermodynamic probability of distribution, obtain the Bose-Einstein distribution law. What are bosons? Give one example. (6+2)

c) Using Maxwell relations derive thermodynamic equations of State. Why is it called 'thermodynamic equations of state'? (6+2)

d) (i) Give the expression for the 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.

(ii) The vibrational frequency and anharmonicity constant of a diatomic molecule are 350 cm^{-1} and 0.0035 respectively. Find out the positions of the fundamental and first overtone band. (1+2+2) +3

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