Roll No. | | | | | | | | | | | | |

Total No. of Pages : 02

Total No. of Questions : 19

M.Sc. (Chemistry)PIT (2015 to 2017) (Sem.–2)

PHYSICAL CHEMISTRY-II(QUANTUM AND STATISTICAL CHEMISTRY)

Subject Code : CHL-413

Paper ID : [51150]

Time : 3 Hrs. Max. Marks : 70

INSTRUCTIONS TO CANDIDATES :

1. **SECTION-A is COMPULSORY consisting of TEN questions carrying TWO marks each.**
2. **SECTION-B contains SIX questions carrying FIVE marks each and students have to attempt ALL questions.**
3. **SECTION-C contains THREE questions carrying TEN marks each and students have to attempt any TWO questions.**

SECTION-A

1. Define Heisenberg uncertainty principle. Give its one significance.

2. Determine whether the following operator is linear or nonlinear :

$$\hat{A}f(x) = x^2 f(x)$$

3. Show that e^{ax} is an eigen function of the operator d^n / dx^n. What is the eigen value?

4. Write down time independent Schrodinger equation of one dimensional harmonic oscillator.

5. Which of the following wave functions are acceptable in quantum mechanics?

$$\psi = \sin x, \psi = \tan x, \psi = \text{cosec } x, \psi = \cos x + \sin x, 0 < x < 2\pi$$

6. Calculate the magnitude of the orbital angular momentum for H-atom for $l = 2$.

7. How many microstates are possible for p^3 configuration?

8. Write down the relation of entropy with the partition function of the system.

9. Write down two differences between bosons and fermions with suitable examples.

10. The molecules of a gas have two energy states 0 and ε and degeneracies g_1 and g_2 respectively. Write down the expression for the molecular partition function.

SECTION-B

11. Calculate the de Broglie wavelength of an electron which has a kinetic energy of 13.6 eV. [leV = 1.602×10^{-19} J; Mass of an electron (me) = 9.1×10^{-31} kg]

12. The wave function for the hydrogen atom is $\varphi = A\, e^{im\varphi}$. Evaluate the normalization constant.

13. Energy of a particle in a cube with dimension L is given by $14h^2/8L^2m$. Calculate the degeneracy.

14. Define heat capacities at constant pressure and constant volume. Mention the relationship between these heat capacities.

15. Compare Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics by giving examples.

16. What is meant by partition function? Write down its significance.

SECTION-C

17. Derive the Huckel MO theory for ethylene/ethene. Draw simple schematics of the bonding and anti-bonding energy level diagrams. Calculate the Bond Orders (B.O.) of O_2^+, O_2 and O_2^- using Molecular Orbital (MO) theory. Which one has the highest bond distance among the above three molecules.

18. What is Bose-Einstein statistics? What are its assumptions? Derive the Bose-Einstein distribution law.

19. Discuss briefly about translational partition function and rotational partition function. Consider 20 molecules divided equally between 4 non-degenerate energy levels. What is the thermodynamic probability (W) for this distribution? How does the value of 'W' change if one molecule is removed from one level and added to another?