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Total No. of Questions : 11

M.Sc (Chemistry) (2018 Batch) (Sem.-2)

PHYSICAL CHEMISTRY - II

Subject Code : CHL-413-18

M.Code : 75983

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 EIGHT questions carrying FIVE marks each and students have to attempt any SIX questions.
3. SECTION-C will comprise of two compulsory questions with internal choice in both these questions. Each question carries TEN marks.

SECTION-A

Q.1 **Answer Briefly**

a. Write down time independent Schrödinger equation and explain all the terms.

b. Check the acceptability of the following function :

$$\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \text{ in the range (0 to L)}$$

c. Determine whether the following operator is linear or nonlinear.

$$\frac{d^2}{dx^2}$$

d. Determine whether the following functions are normizable or not over the indicated intervals :

$$\text{Sin } x \ (0, \pi)$$

e. Why the value of $\psi^*\psi$ be finite everywhere?

f. Show that if the linear operators A and B have common complete set of eigen functions, then A and B commute.

g. For a particle in a cubical box what is the degeneracy of the level that has energy 14/3 times that of the lowest level?

h. Write the ground state term symbols for the following electronic configurations of $3d^2$ and $2p^3$.

i. Calculate the number of radial node and angular node of 5d orbital.

j. Calculate the momentum of a photon having wavelength 200 nm.

SECTION-B

2. The wave function ψ of a certain system is a linear combination of following : $\psi = \sqrt{\frac{1}{2}}\psi 1 + \sqrt{\frac{3}{2}}\psi_2$, where ψ_1 and ψ_2 are the eigen functions with eigen value E_1 and E_2. What is probability that the system energy will be observed to be E_2?
3. Show that the function $\psi = xe^{-ax^2}$ is an eigen function of the operator $\frac{d^2}{dx^2} - 4a^2x^2$. What is its eigen value?
4. Calculate the probability that a particle in 1-D box of length L is found between 0 and L/2.
5. Determine the value of A_m so that the wave function $\psi_m(\phi) = A_m e^{im\phi}$, where, m = 0, ±1, ±2 $(0 \le \phi \le 2\pi)$ are normalized.
6. A particle in one dimensional box simple harmonic oscillator in x-direction is perturbed by a potential λx. What is the 1st order correction for ground state?
7. Find out $\langle P_x \rangle$ for a harmonic oscillator in its ground state.
8. Write a short note on Russel-Saunders (R-S) coupling.
9. Arrange the following states (term symbols) for p^2 configuration in the increasing order of energy : ^1D, ^3P and ^1S. Justify the trend of the result.

SECTION-C

10. The radial function for a 2s electron in hydrogen atom is given by :

$$R_{2s} = \frac{1}{\sqrt{2}}\left(\frac{1}{a_0}\right)^{3/2}\left(1 - \frac{r}{2a_0}\right)e^{-r/2a_0}.$$

Determine the number and location of node(s) in the 2s wave function. Plot the plot of R_{2s} against 'r' and also the radial distribution plot for R_{2s}.

OR

10. Write the electronic Hamiltonian of a hydrogen molecule ion (H_2^+) and explain each term briefly and clearly with the help of a schematic diagram.
11. Derive the Huckel MO theory for ethylene. Draw simple schematics of the bonding and anti-bonding energy level diagrams.

OR

11. Describe the variation theory and prove the same in detail.

NOTE : Disclosure of Identity by writing Mobile No. or Making of passing request on any page of Answer Sheet will lead to UMC against the Student.