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## M.Sc. (Chemistry) (2018 Batch) (Sem.-2) PHYSICAL CHEMISTRY - II Subject Code : CHL-413-18 M.Code : 75983 Date of Examination : 16-12-22

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**

#### 1. Answer briefly :

a) Which of the following wave functions are acceptable in quantum mechanics

 $\Psi = \sin x, \Psi = \tan x, \Psi = \operatorname{cosec} x, \Psi = \cos x + \sin x, 0 < x < 2\pi.$ 

- b) Determine whether the following operator is linear or nonlinear : SQRT (where, SQRT = square root).
- c) Show that  $e^{ax}$  is an eigen function of the operator  $d^n/dx^n$ . What is the eigen value?
- d) Calculate the magnitude of the orbital angular momentum for H-atom for l = 2.
- e) How many microstates are possible for  $p^3$  configuration?
- f) Check the acceptability of the following function :  $\sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$  n the range (0 to a),
- g) How many microstates are possible for  $p^3$  configuration?
- h) Write down time independent Schrodinger equation and explain all the terms.
- i) Calculate the number of radial node and angular node of 5d orbital.
- j) What is the complex conjugate of the wave function  $(\psi 6i)$ ?

#### **SECTION-B**

- 2. Briefly describe the quantum mechanical postulates with proper explanation.
- 3. Write a short note on Russel-Saunders (R-S) coupling.
- 4. If two operators  $\alpha$  and  $\beta$  are Hermitian, find out the condition that their product  $\alpha\beta$  will also be Herpnitian.
- 5. Prove that position and momentum operator do not commute.
- 6. The energy of particle 3d box is  $E = 25h^2/8mL^2$ . How many degenerate states are prossible? Write down the degenerate states.
- 7. Write a short note on Hamiltonian operator.
- 8. Arrange the following states (term symbols) for  $p^2$  configuration in the increasing order of energy: 3P and with proper explanation.
- 9. Calculate the degeneracies of a particle of mass m in a 3-D cubical box of width L having energies equal to 9 in units of  $(h^2/8mL^2)$ .

## **SECTION-C**

10. Derive the Huckel MO theory for 1,3-butadiene. Draw simple schematics of the bonding and anti-bonding energy level diagrams.

#### OR

The wave function  $\psi$  of a certain system is a linear combination of following:  $\psi = \sqrt{\frac{1}{4}} \psi_1 + \sqrt{\frac{3}{4}} \psi_4$ , where  $\psi_1$  and  $\psi_2$  are the eigen functions with eigen value  $E_1$  and  $E_2$ . What is probability that the system energy will be observed to be  $E_1$ ?

11. Briefly describe the perturbation theory.

## OR

Write Schrodinger equation for motion of an electron in a Hydrogen like atom in spherical coordinates. Separate the equation into three functions  $R(r)Y(\theta)Z(\phi)$  and solve.

# 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.