

Unit IV

No. of Printed Pages : 04

Roll No.

7. Describe in detail linear combination of atomic orbital methods to predict :

- (i) Symmetric and anti symmetric wave functions of molecular orbital
- (ii) Energy of hydrogen molecules ion. **10,10**

8. Write short notes on the following :

- (a) Hybridization
- (b) Influence of spin on wave function of atoms. **10,10**

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M. Sc. EXAMINATION, May 2017

(Third Semester)

(Re-appear Only)

CHEMISTRY

CH-627-B

Physical Chemistry Special-II

(Quantum Chemistry)

Time : 3 Hours]

[Maximum Marks : 100

Before answering the question-paper candidates should ensure that they have been supplied to correct and complete question-paper. No complaint, in this regard, will be entertained after the examination.

Note : Attempt *Five* questions in all, selecting at least *one* question from each Unit. All questions carry equal marks.

Unit I

1. (a) Prove that $[\hat{j}_+, \hat{j}_-] = 2\hbar\hat{j}_z$. **8,12**
(b) Prove that the eigen values of \hat{j}_z operated on function $\Psi_{j,m}$ yields eigen value $m\hbar$.
2. (a) Derive expression for operator of angular momentum in Cartesian coordinates. **6**
(b) $[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$ **7**
(c) Prove that step down Ladder operator lowers the eigen values of \hat{j}_z by \hbar .

Unit II

3. (a) What happened to the particle, if the walls of 3-D box removed ? **4**
(b) Explain the solution of angular equation for H-atom. **8**
(c) What do you know about the quantization of energy of microscopic particle ? **4**
(d) Explain the zero point energy of particle when in :
(i) Simple Harmonic oscillator system
(ii) Rigid Rotator system. **4**

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4. (a) What happened in energy levels when ?
(i) mass of particle increases in 3-D box
(ii) Length of 3-D box decreases. **6**
(b) Calculate the average distance of 2s electron from nucleus of hydrogen atom. **6**
(c) Explain the equation of :
(i) Hermite polynomial
(ii) Laguerre polynomial. **4 each**

Unit III

5. Describe variation principle. How this can be utilized to find the energy of Helium atom ? **20**
6. State and explain first order perturbation theory. Utilize it to an electron in a onedimensional box under the influence of electric field. **20**

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P.T.O.