2019/EVEN/CHMH–603/237

TDC Even Semester Exam., 2019

CHEMISTRY

(Honours)

(6th Semester)

Course No. : CHMH–603

(Physical Chemistry)

Full Marks : 35
Pass Marks : 12

Time : 2 hours

The figures in the margin indicate full marks for the questions

Answer **five** questions, taking **one** from each Unit

UNIT—I

1. *(a)* Using LCAO-MO method for the wavefunction for H_2, obtain the normalized wavefunction for bonding and anti-bonding molecular orbitals. 4

(b) Write the molecular orbital configuration of the species O_2, O_2 and O_2. Which of these species would have the maximum bond strength? 3

2. *(a)* Consider the case of H_2 molecule in terms of VBT to give the symmetric and anti-symmetric wavefunctions and energy levels. 5

(b) Build the Hamiltonian for hydrogen molecule using MOT, giving the meaning of the terms involved. 2

UNIT—II

3. *(a)* State and explain Einstein's photoelectric equation. 2

(b) Set up and solve the Schrödinger wavefunction for a particle in an infinite one-dimensional box with potential energy zero inside the box. Normalize the wavefunction. 5

4. *(a)* Derive the de Broglie equation and verify it experimentally. 1+2=3

(b) A cricket ball weighing 100 g is to be located within 0·1 Å. What is the uncertainty in its velocity? Comment on your result. 2

(c) Verify that the wavefunction of particle in a one-dimensional box of width *a* and infinite height are orthogonal. 2

UNIT—III

5. *(a)* Verify the Heisenberg uncertainty principle for the ground state of a one-dimensional simple harmonic oscillator. 5

(b) Show that the 1s wavefunction of hydrogen atom is given by

$$_{1s} \quad \frac{1}{\sqrt{\ } \, a_0^{3/2}} \, e \qquad \frac{r}{a_0}$$

a_0 is the Bohr radius. 2

6. *(a)* Set up the Schrödinger wavefunction for a simple harmonic oscillator and solve it for the energy eigenvalues. 5

(b) Using the normalized wavefunction

$$_{1s} \quad \frac{1}{(\; a_0^{3})^{1/2}} \, e \qquad \frac{r}{a_0}$$

for the ground state of hydrogen atom, calculate the probability for the electron to be confined in a sphere of radius $r \quad a_0$, the Bohr radius. 2

UNIT—IV

7. *(a)* State Hückel's $4_{n} \;\; _{2}$ rule of aromaticity. Illustrate giving two specific examples. 2

(b) Set up and solve the Hückel secular equation for ethylene system and calculate the -bond energy in ethylene. Show the results on the HMO diagram. 4+1=5

8. *(a)* Set up the Hückel secular equation for cyclobutadiene. Calculate the energies of the -orbitals and determine the delocalization energy. 4

(b) Compare among the stabilities of cyclopentadiene cation, anion and radical using Hückel theory for cyclic conjugated systems and aromaticity. 3

UNIT—V

9. *(a)* Derive Debye T-cubed law for the heat capacity of a crystal. 4

(b) Calculate the translation partition function for hydrogen atom at 3000K confined to move in a box of volume of $2 \;\, 494 \quad 10^{5}\ \mathrm{cm}^{3}$. Also determine the thermal de Broglie wavelength. 2+1=3

10. *(a)* Using the concept of molecular partition function, show that for an ideal monoatomic gas $PV = nRT$ which is the ideal gas equation. 4

(b) For H_2 gas at 3000K, calculate the characteristic vibrational temperature and the vibrational partition function given that the fundamental frequency of H_2 molecule is $4405 \cdot 3\ cm^{-1}$. 3

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