

Veer SurendraSai University of Technology

Department of Chemistry

Mid Term Examination November 2015

1<sup>st</sup> Semester B. Tech. (Section-H, I, J, K, L, M, N)

Sub: Chemistry -I

Max. Marks: 20

Time: 2 Hrs.

Note: Q. No. 1 is Compulsory Answer any three from the rest of the questions

1.

[1x5=5]

- a) Write the conditions for a valid wave functions; the solution to Schrodinger's wave equation.
- b. An electron is confined in a one-dimensional box of length 1 Å. Calculate the ground state energy of the electron.
- c) Write the conditions for a molecule to be microwave and IR active.
- d. 2 M solution of a compound transmits 30% of the incident radiation of wavelength 400 nm in a cuvette of 1 cm width. Calculate the molar absorptivity of the solution.
- e) State Frank-Condon principle.
2. a) When a radiation of certain wavelength is incident on a metallic surface, the stopping potential is found to be 4.8 V. If the same surface is illuminated by the radiation of double the wavelength, the stopping potential is found to be 1.6 V. What is the threshold wavelength of the surface? [2.5]
- b) Briefly describe absorption, fluorescence, phosphorescence using Jablonski diagram. [2.5]
3. Derive the complete wave function and total energy for a particle of mass 'm' moving in a one-dimensional box of length 'l' using Schrodinger time-independent wave equation. [5]
- X a) The fundamental vibrational frequency of HCl is  $8.5 \times 10^3 \text{ s}^{-1}$ . Calculate the force constant of the molecule if mass of H is 1.008 g/mole and that of Cl is 35.5 g/mole. [2.5]
- b) Discuss the basic principle and types of electronic transition in UV-Visible spectroscopy. [2.5]
5. a) The first line in the pure rotational spectrum of  $^1\text{H}^{35}\text{Cl}$  appears at  $21.18 \text{ cm}^{-1}$ . Find out the rotational constant of  $^2\text{D}^{35}\text{Cl}$ . Given atomic masses of H, D and Cl are 1.008 amu, 2.015 amu and 35.45 amu, respectively. Assume, bond length in  $^2\text{D}^{35}\text{Cl}$  is same as that in  $^1\text{H}^{35}\text{Cl}$ . [2.5]
- b) Calculate the voltage required to accelerate an electron to have a velocity of  $1.87 \times 10^6 \text{ m.s}^{-1}$ . What will be the de-Broglie wavelength? [2.5]
6. a) Write the selection rule for rotational spectroscopy and IR spectroscopy (for a harmonic and an-harmonic oscillating molecule). [2.5]
- b) The pure rotational spectrum of  $^{12}\text{C}^{14}\text{N}$  molecule consists of a series of equally spaced lines separated by  $20.80 \text{ cm}^{-1}$ . Calculate the inter-nuclear distance of the molecule. [2.5]