(c) The fundamental vibrational frequency of HCl is 2890 $cm^{-1}$. Calculate the force constant of this molecule. (5,5,5)



[This question paper contains 8 printed pages.]

**Your Roll No.....**

**Sr. No. of Question Paper : 5855** **J**

Unique Paper Code : 2172513601

Name of the Paper : DSC: QUANTUM CHEMISTRY AND SPECTROSCOPY

Name of the Course : **BACHELOR OF SCIENCE PHYSICAL SCIENCES WITH CHEMISTRY**

Semester : VI

Duration : 2 Hours Maximum Marks : 60

**Instructions for Candidates**

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt any **four** questions.
3. Scientific calculator is permitted.

**Physical Constants**

Mass of electron, $m_e = 9.1 \times 10^{-31}$ kg

Velocity of light, $c = 3.0 \times 10^{8} ms^{-1}$

Planck's constant, $h = 6.626 \times 10^{-34} Js$

Atomic mass of $H^1 = 1.673 \times 10^{-27}$ kg

Atomic mass of $Cl^{35} = 58.06 \times 10^{-27}$ kg

Atomic mass of $C^{12} = 1.99 \times 10^{-26}$ kg

Atomic mass of $O^{16} = 2.66 \times 10^{-26}$ kg

1. (a) What are the postulates of quantum mechanics?

   (b) Derive Schrodinger wave equation.

   (c) Derive the expression for energy of a particle in one-dimensional box. (5,5,5)



   (i) $C_2H_6$

   (ii) $C_2H_2$

   (iii) $C_2H_4$

   (c) Briefly explain the fluorescence and phosphorescence using Jablonski diagram. (5,5,5)

6. (a) What is the difference between atomic and molecular spectra?

   (b) The inter molecular distance of carbon monoxide molecule is $1.13 \times 10^{-10}$ m. Calculate the energy (in joules) of this molecule in the first exited rotational level.

(ii) $H_2O$

(iii) $C_6H_6$

(iv) $CHCl_3$

(v) $O_2$ (5,5,5)

5. (a) What is the effect of hydrogen bonding (inter- and intramolecular) on vibrational frequencies (IR frequencies) of molecules? Explain with suitable examples.

(b) What is the influence of Inductive effect on IR frequencies of organic molecules? Arrange the following molecule according to increasing order of its C-H stretching frequencies.



2. (a) What is the ground state energy for an electron which is confined to a potential well (one-dimensional box) having a width of 0.2 nm.?

(b) Calculate the transmittance, absorbance and absorption coefficient of a solution which absorbs 90% of a certain wavelength of light beam passed through a 1 cm cell containing 0.25 M solution.

(c) The pure rotational (microwave) spectrum of gaseous HCl consists of a series of equally spaced lines separated by 20.80 $cm^{-1}$. Calculate the intermolecular distance of the molecule.

(5,5,5)

3. Write short note on **any three** of the following :

(a) Chromophores and Auxochromes

(b) Bathochromic and Hypsochromic shifts

(c) Born- Oppenheimer approximation

(d) Lambert-Beer's law (5,5,5)

4. (a) Which of the following molecules will show a vibrational infrared spectrum and why?

(i) $Cl_2$

(ii) HCl

(iii) $CH_3Cl$

(iv) $C_6H_6$

(v) $NH_3$



(b) Which of the following molecules will show a pure rotational spectrum and why?

(i) $H_2$

(ii) HBr

(iii) $C_2H_6$

(iv) $C_6H_6$

(v) $H_2O$

(c) How many fundamental vibrational frequencies (i.e. fundamental vibrational degrees of freedom) are expected for the following molecules.

(i) $CO_2$