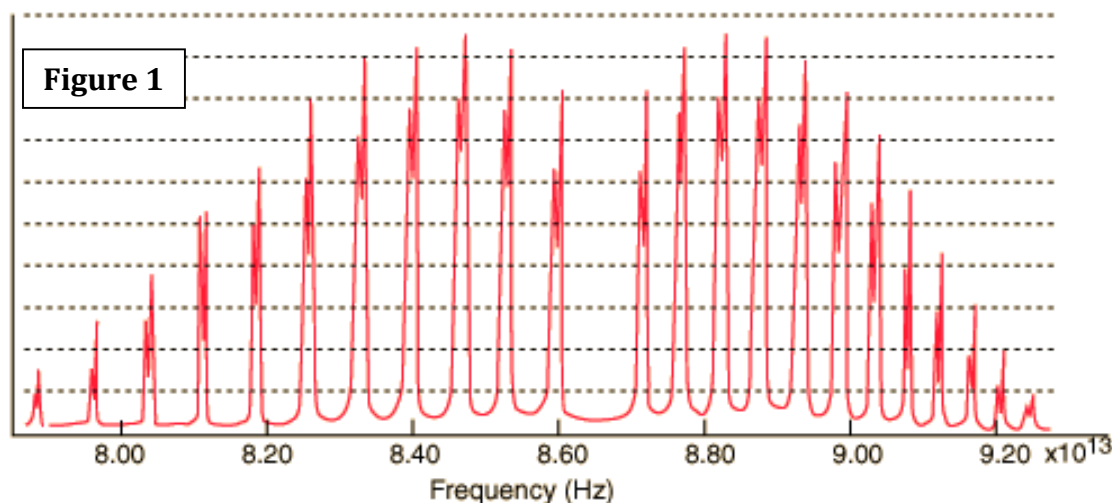


INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH, MOHALI
CHM201: SPECTROSCOPIC AND OTHER PHYSICAL METHODS

Constants: $N = 6.023 \times 10^{23} \text{ mol}^{-1}$; $k = 1.381 \times 10^{-23} \text{ JK}^{-1}$; $h = 6.626 \times 10^{-34} \text{ Js}$;
 $c = 3 \times 10^8 \text{ ms}^{-1}$; Rel. atomic weight of H = 1.000; absolute mass of H-atom = $1.67343 \times 10^{-27} \text{ kg}$.

1. An experimental Rotation-Vibration spectrum of $^1\text{H}-^{35}\text{Cl}$ for $v = 0$ to $v = 1$ transition is shown in Figure 1 and the corresponding band positions are given below:

$P_0 = 8.60 \times 10^{13} \text{ Hz}$; $R_1 = 8.70 \times 10^{13} \text{ Hz}$



- (a). Calculate the (i) rotational constant (in cm^{-1}), (ii) equilibrium bond length (nm), (iii) anharmonicity constant and (iv) force-constant (pN/nm) of $^1\text{H}-^{35}\text{Cl}$ from the spectrum. [Given the equilibrium oscillation frequency, $\bar{\omega}_e = 2990 \text{ cm}^{-1}$]

$$2.5 + 2.5 + 2.5 + 2.5 = 10$$

2. a. Which of the following molecules may show a pure rotational microwave spectrum:

(i) H_2 , (ii) HCl , (iii) CH_4 , (iv) H_2O

b. If the equilibrium oscillation frequency of CO is, $\overline{\omega_e} = 2990 \text{ cm}^{-1}$, $\overline{\omega_e} * x_e = 52 \text{ cm}^{-1}$ and the equilibrium dissociation energy (D_e) is 35486 cm^{-1} . Calculate the experimental dissociation energy (D_0). **3**

c. Draw schematically the pure rotational energy levels of rigid $^{12}\text{C}^{16}\text{O}$ and compare it with $^{13}\text{C}^{16}\text{O}$. Extend this comparison for non-rigid $^{13}\text{C}^{16}\text{O}$ on the same energy diagram. **5**

2. Each question contains (+2) marks for correct answer and (-2) marks for wrong answer. Fill the correct circle with pen of any color.

$$10 \times 2 = 20$$

a) In Figure 1, we observe doublets for P and R bands and these doublets are due to the fact that:

- ☐ $^1\text{H}-^{35}\text{Cl}$ is a non-rigid rotor;
- ☐ The transition is associated with vibrational transition;
- ☐ The sample of $^1\text{H}-^{35}\text{Cl}$ is naturally mixed with $^1\text{H}-^{37}\text{Cl}$;
- ☐ $^1\text{H}-^{35}\text{Cl}$ is a rigid rotor;

b) In FT-IR spectroscopy, we do Fourier transform of the data as

- ☐ Temporal function to frequency function
- ☐ Interferogram to frequency function
- ☐ Frequency function to Interferogram
- ☐ Temporal function to wavelength function

c) The lifetime of a state that gives rise to a line of width 1 cm^{-1} is

- ☐ 5 ps
- ☐ 5 ns
- ☐ 10 ns
- ☐ 1 ns

d) Role of a grating in a spectrometer is to

- ☐ Steer monochromatic beam in different directions
- ☐ Disperse white light into different wavelengths
- ☐ Count no of photons falling on detector
- ☐ Focus the incident radiation to sample

e) The peak maxima for any rotational spectrum

- ☐ appears at $J=0$ to $J=1$ transition always
- ☐ Is dependent on molecules under probe
- ☐ Is dependent on the ground state of v
- ☐ Is random

f) The molecule $^{16}\text{O}-^{18}\text{O}$ is microwave-active,

- ☐ Always
- ☐ Only when associated with vibrational transitions
- ☐ Never
- ☐ Only when the incident radiation is along the principle rotational axis of the molecule

g) The peak maxima for any vibrational spectrum

- ☐ appears at $v=0$ to $v=1$ transition always

- ☐ Is dependent on molecules under probe
 - ☐ Is random
 - ☐ None of the above
- h) Blue sky is fact of
- ☐ Mie scattering
 - ☐ Raman scattering
 - ☐ Rayleigh scattering
 - ☐ Tyndall effect
- i) Absorbance (A) higher than 2 is
- ☐ Desirable as it makes the measurement more efficient
 - ☐ Not desirable as only a small fraction of light transmitted to detector
 - ☐ Desirable otherwise detector cannot detect molecules
 - ☐ Not desirable as detector goes blind with such a high intensity of light
- j) A biker is approaching a traffic light at a speed of 6.4×10^7 m/s and as a consequence he sees a red light (660 nm) as a green (520 nm). This is because of
- ☐ Doppler effect
 - ☐ Line-broadening
 - ☐ It is not possible to see red as green
 - ☐ Red and green are kept so closely in the traffic light

ROUGH WORK

ROUGH WORK