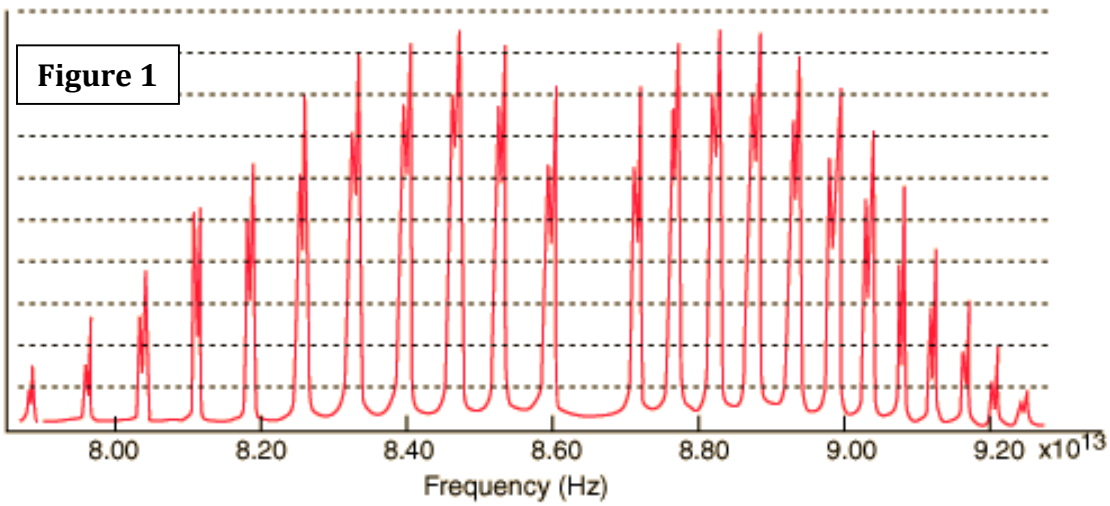
INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH, MOHALI
CHM201: SPECTROSCOPIC AND OTHERR PHYSICAL METHODS

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

1. An experimental Rotation-Vibration spectrum of ^{1}H-^{35}Cl for $v = 0$ to $v = 1$ transition is shown in Figure 1 and the corresponding band positions are given below:
   $P_0 = 8.60*10^{13}$ Hz ; $R_1 = 8.70*10^{13}$ Hz

Figure 1



(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}H-^{35}Cl from the spectrum. [Given the equilibrium oscillation frequency, $\overline{w_e}$ =2990 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: 2

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

b. If the equilibrium oscillation frequency of CO is, $\overline{w_e}$ = 2990 cm^{-1}, $\overline{w_e}*x_e$ = 52 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 $^{12}C^{16}O$ and compare it with $^{13}C^{16}O$. Extend this comparison for non-rigid $^{13}C^{16}O$ 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*2 = 20

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

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

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

- ○ Temporal function to frequency function
- ○ Interferrogram to frequency function
- ○ Frequency function to Interferrogram
- ○ 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}O-^{18}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

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