Ex5a

Exercise 13

13.1 Rigid Rotor and molecular rotations

A molecule oscillates rapidly compared to its rotation. Under this approximation, one can approximate the molecular bond length to be fixed. This is called the Rigid Rotor model.

1. For a diatomic molecule, determine the hamiltonian describing the rotational transitions and show that its eigenvalues are given by

$$E_N = hcBN(N+1) \tag{1}$$

   where the rotational constant B=$\hbar^2/2Ihc$, I is the moment of inertia and N is the quantum number assosciated with the eigenstate.

2. For the a Hydrogen molecule and Hydrogen Chloride molecule, determine these energy levels (Use values of bond length as 0.074 nm for hydrogen molecule and 0.1275 nm for HCl)

3. Plot the population distribution of the above states at 298K and 373K.

4. Isotopologues are molecules that differ only in their isotopic composition. For H_2 , H-D and D_2 , determine the variation in their rotational constant.

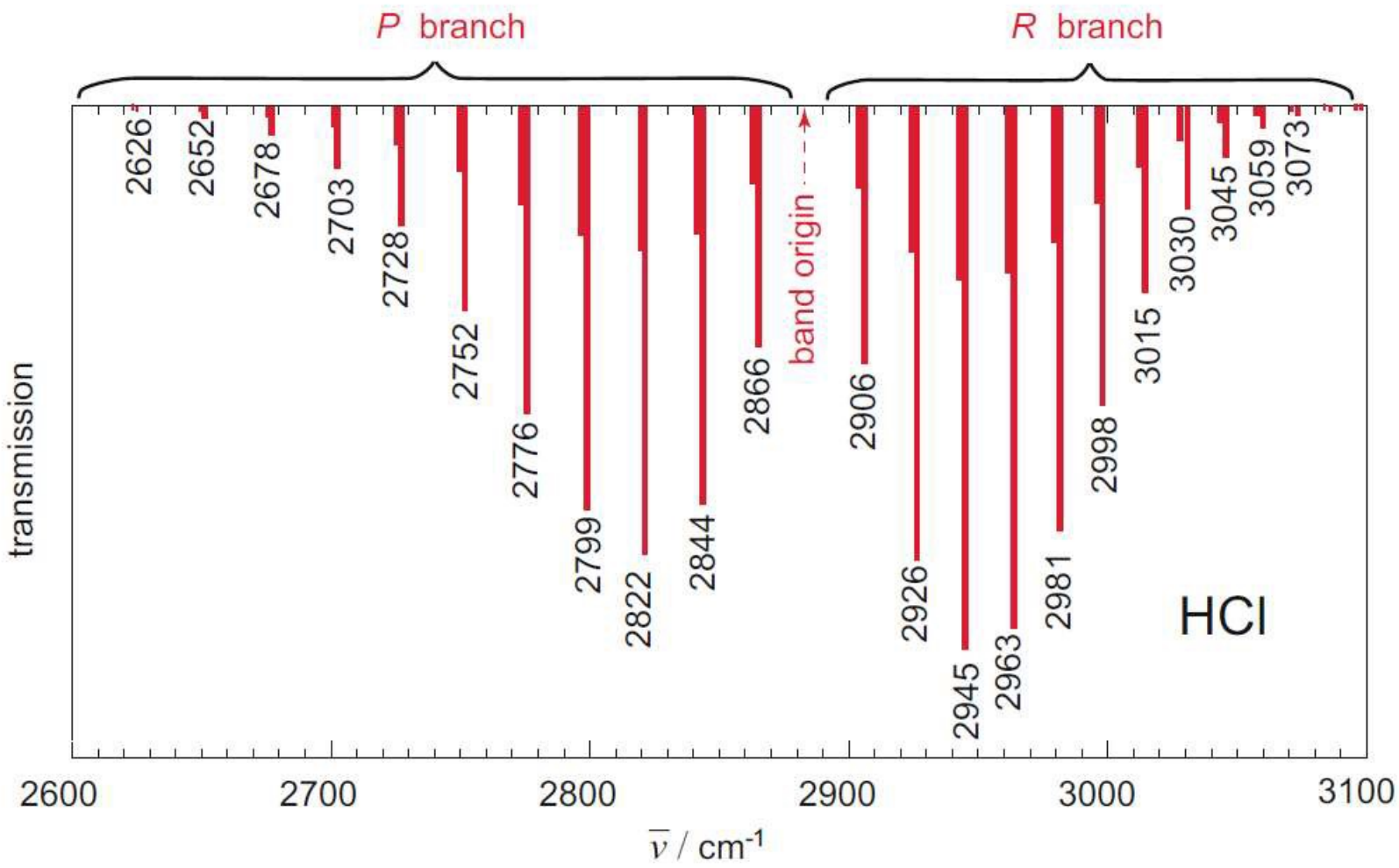
5. Determine the selection rules for E1 transitions.

13.2 Molecular Vibrations and Transitons

1. It is observed that H_2, O_2, are transparent in IR regime while HCl is absorbant. Explain why.

2. Determine the number of modes of vibration of a linear molecule and a non-linear molecule, given that the number of atoms they have is N_a

3. E1 Roto-vibrational transitions in diatomic molecules have the following selections rules : $\Delta N = \pm 1$, $\Delta v = \pm 1$. The transitions ΔN = -1 are called the P-branch and $\Delta N = +1$ are called the R-branch. Can you determine the bond length from the molecular spectra? What about the harmonic frequency?



Vibration-rotation spectrum of HCl, simulated according to HITRAN (ROTHMAN et al. 2009) for absorption at room temperature

Taken from - Ingolf V. Hertel, Claus-Peter Schulz (auth.) - Atoms, Molecules and Optical Physics 2_ Molecules and Photons - Spectroscopy and Collisions (2015, Springer-Verlag Berlin Heidelberg)