Problem set 5

(Will be discussed in the Tutorial session on Oct 8, 2018, 6PM)

1. The R(0) line in the robvibrational spectrum of $^{1}H^{35}Cl$ occurs at 2905.8 cm^{-1}. Calculate the position of the R(0) line for $^{1}H^{37}Cl$ and $^{2}H^{35}Cl$. (Calculate the isotope shift in the vibrational frequency.)

2. Using the rovibrational spectrum of the HCl (given below), calculate B_0 and B_1 (rotational constants in the v=0 and v=1 levels). Also calculate r_0 and r_1 for the two vibrational states. (Use combination differences)

3. Using the B_0 and B_1 values you calculated in problem 2, calculate the J value at which a turn around of the rotational branch will occur, to form a head. Which branch, P or R, will show a turn around and form a head?

4. If the *difference* between B_0 and B_1 was ten times larger than what you calculated in problem 3, at what value of J will a head be formed.

5. I_2, in its ground electronic state, ***X***, has a vibrational frequency of 212 cm^{-1} and an $\boldsymbol{R_e}$ of 2.66 Å. In an excited electronic state, ***B***, it has the following properties: vibrational frequency of 125 cm^{-1} and an $\boldsymbol{R_e}$ of 3.03 Å. In yet another electronic state, ***a***, it has the following parameters: vibrational frequency of 205 cm^{-1} and an $\boldsymbol{R_e}$ of 2.75 Å. Transitions are observed between $\boldsymbol{X \rightarrow B}$ and $\boldsymbol{X \rightarrow a}$. Which of these two transitions is likely to show a *long* progression of vibrational bands? Justify your answer.

6. If the rotational structure in the vibrational bands were to be analysed in both the above transitions, what would you observe – red degraded band heads or violet degraded band heads? Why? In which of those two transitions, $\boldsymbol{X \rightarrow B}$ or $\boldsymbol{X \rightarrow a}$, would the turning around of the rotational lines occur at a lower J value?

7. The Na atom has a strong line corresponding to a transition between the ^{2}S and ^{2}P states. This line has been observed to be a doublet. Explain why this line occurs as a doublet.

8. Draw the energy level diagram for He (including both singlet and triplet states) and show the transitions that are allowed.