

**CHM201**

**Problem set 2**

**(Rotational spectroscopy)**

(Will be discussed in the Tutorial session)

In all the calculations, where the speed of light,  $c$ , is required, assume it to be  $2.9979 \times 10^{10} \text{ cm s}^{-1}$

1. In a certain experiment, the rotational constant  $B$  for  $^{12}\text{C}^{16}\text{O}$  was determined to be  $1.929 \text{ cm}^{-1}$ . Using this value for  $B$ , calculate the bond length in CO. Another researcher repeats the experiment and reports a  $B$  value of  $3.858 \text{ cm}^{-1}$  for CO. Can you pass a judgement on who is more likely to be correct and if any of the values of  $B$  is clearly indicated to be incorrect?
2. The  $B$  value for HF is  $20.56 \text{ cm}^{-1}$ .
  - a) For this molecule calculate the populations, relative to that in  $J=0$ , for the  $J$  levels upto 10 and plot a histogram showing the population. What is the  $J$  level where the population is the highest? Does this  $J$  value with the highest population, agree with the calculation of the most probably  $J$  that you calculate from the equation derived in class. Assume the temperature to be 300 K.
  - b) Repeat the above calculation for the temperatures 50 K and 600 K. This will help you understand the effect of temperature.
3. The  $B$  value for HI is  $6.43 \text{ cm}^{-1}$ .
  - c) For this molecule calculate the populations, relative to that in  $J=0$ , in the  $J$  levels upto 10 and plot a histogram showing the population. What is the  $J$  level where the population is the highest? Does this  $J$  value with the highest population, agree with the calculation of the most probably  $J$  that you calculate from the equation derived in class. Assume the temperature to be 300 K.
  - d) Repeat the above calculation for the temperatures 50 K and 600 K. This will help you understand the effect of temperature.

(Comparing the results of problem 2 and 3 will help you understand the distribution of population in various levels as a function of  $B$  values. )