

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 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 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 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 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.)