Chemistry 432
Problem Set 6
Spring 2021

1. The boron fluoride molecule has a bond length of 1.26 Å and a fundamental vibrational frequency of 1402.1 cm^{-1}. Calculate the relative intensities of the rotational-vibrational absorption spectral lines of the P-branch transition originating in state $n = 0, J = 1$ to the R-branch transition originating in state $n = 0, J = 0$ at 298K.

2. In the gas phase the the first two lines of the R branch of the rotation-vibration spectrum of BrCl occur at 444.58 cm^{-1} and 444.88 cm^{-1}. Calculate the force constant and the bond length of the BrCl molecule in the gas phase.

3. The vibrational frequency of the CaH molecule in the gas phase is 3.892 $\times 10^{13}$ s^{-1}, and the bond length of CaH in the gas phase is 2.002 Å. Calculate the frequency of the first line in the R-branch of the rotational-vibrational spectrum of gas phase CaH.

4. The first two lines in the P branch of the infrared vibration-rotation spectrum of the gas-phase SnTe molecule occur at 259.4406 cm^{-1} and 259.3544 cm^{-1}. Calculate the bond length of SnTe and the vibrational frequency of the SnTe molecule in the gas phase.

5. The first two lines in the R branch of the rotational-vibrational spectrum of the gas-phase BN molecule are measured to be 1517.9 cm^{-1} and 1521.3 cm^{-1}. Calculate the bond length and natural frequency of vibration of BN in s^{-1} in the gas phase.

6. The frequencies of the first two lines in the R branch of the rotational-vibrational spectrum of the gas-phase AlF molecule occur at 803.4 cm^{-1} and 804.5 cm^{-1}‘. Calculate the natural frequency of vibration and the bond length of AlF.

7. The first two lines in the R-branch of the vibration-rotation absorption spectrum of the HF molecule occur at 4180.58 cm^{-1} and 4222.83 cm^{-1}. Calculate the bond length and force constant of the HF molecule.

8. The pure rotational Raman spectrum of N_2 shows a series of lines with uniform spacing of 7.99 cm^{-1}. Calculate the bond length of the N_2 molecule.

9. The carbon monoxide molecule has a bond length of 1.128 Å and a natural vibrational frequency of 2169.8 cm^{-1}. Calculate the frequency shifts of the first O-branch the Q-branch and the first S-branch transitions in the rotational-vibrational Raman spectrum of CO.

10. The first two lines in the R branch of the vibrational-rotational spectrum of the gas-phase BH molecule occur at 2390.9 cm^{-1} and 2415.0 cm^{-1}. In a Raman experiment light of wavelength 5723. Å is scattered from a sample of BH gas. Calculate the frequency in units of s^{-1} of the first line in the O branch of the vibrational-rotational Raman spectrum.

11. Light of frequency 5.9960 $\times 10^{14}$ s^{-1} is scattered from PtO molecules in the gas phase. The Stokes, Q-branch line in the rotational-vibrational Raman spectrum from the scattered light is observed at 5.7408 $\times 10^{14}$ s^{-1} and the first Stokes, O-branch line is observed at 5.7415 $\times 10^{14}$ s^{-1}. Calculate the bond length and Hooke's Law vibrational force constant for PtO in the gas phase.

12. The frequency shift of first line in the O branch of the rotational-vibrational Raman spectrum of the gas-phase iodine oxide molecule (IO) occurs at $\nu_{out} - \nu_{in} = -2.037 \times 10^{13} s^{-1}$, and the frequency shift of the first line in the S branch of the same molecule occurs at $\nu_{out} - \nu_{in} = -2.049 \times 10^{13} s^{-1}$. Calculate the bond length of the IO molecule in the gas phase.

13. When visible light of frequency 5.996000 $\times 10^{14}$ s^{-1} scatters off the gas-phase GeS molecule, the first two lines in the O branch of the vibrational-rotational Raman spectrum occur at 5.903307 $\times 10^{14}$ s^{-1} and 5.903532 $\times 10^{14}$ s^{-1}. Calculate the bond length and harmonic vibrational frequency in s^{-1} of the GeS molecule.