CHEM106: Assignment 11

Microwave, IR, and Raman Spectra

1. Which of the following molecules are microwave active? Indicate the reason for your choice.

A. F2; not active

B. NO; active

C. CH3I; active

D. CO2;not active

According to the gross selection rule, the molecule must possess a permanent dipole moment for a rotational transition in the microwave spectroscopy.

2. Which of the following vibrational modes of the carbon dioxide molecule CO2 will be IR active? Which will be Raman active?



To be IR active, there must be a change in dipole moment as the molecule undergoes vibrational motion. So the v2 and v3 modes of vibration are IR active.

To be Raman active, there must be a change in polarizability as the molecule undergoes vibrational motion. So the v1 mode of vibration is Raman active.

3. The spacing between the lines in the microwave spectrum of H19F is 41.9 cm-1. Calculate the bond length of the H19F molecule.

Spacing in the microwave spectrum equals to 2B (in Hz), where . We also know that the moment of inertia , where is the reduced mass,

.

At first, we need to express the line spacing in unit of Hz:

.

Next, we need to figure out the moment of inertia I:

.

Finally, Å.

4. The fundamental vibrational frequency of H127I is 2309.5 cm-1. Calculate the force constant for the stretching vibration of the H127I molecule.

The vibrational frequency  is related to the force constant k by the relationship , where is the reduced mass,

.

We also know that .

Therefore,

.

5. Determine the number of normal mode vibrations in the following molecules.

A. HCl; For a linear molecule, the number of normal modes of vibration is

3N – 5 = 6 – 5 = 1.

B. C6H6; For a nonlinear molecule, the number of normal modes of vibration is

3N – 6 = 36 – 6 = 30.

C. CHCl3; For a nonlinear molecule, the number of normal modes of vibration is

3N – 6 = 15 – 6 = 9.

D. CO2; For a linear molecule, the number of normal modes of vibration is

3N – 5 = 9 – 5 = 4.