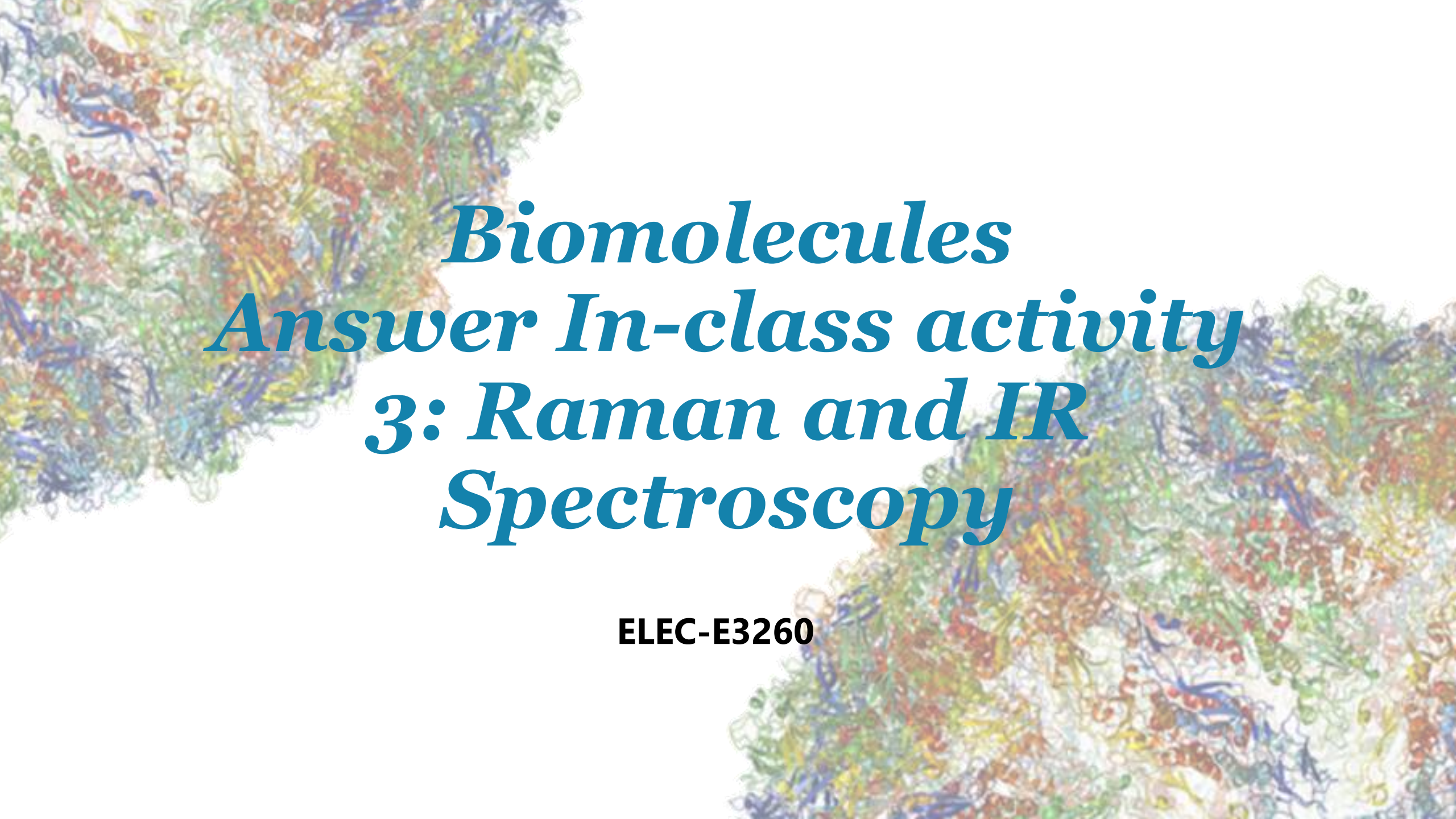


Biomolecules Answer In-class activity 3: Raman and IR Spectroscopy

ELEC-E3260

In-Class Activity

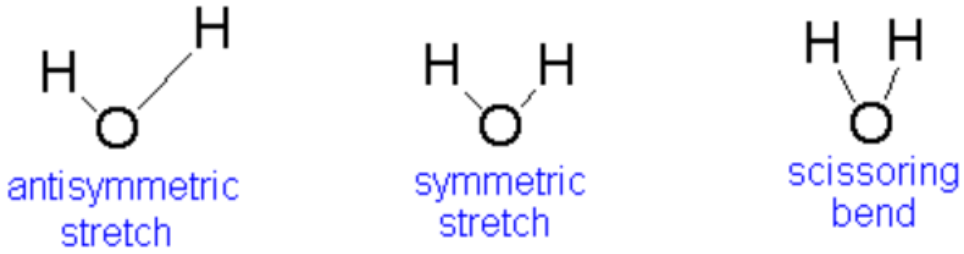
1. Give me the number of Normal Vibrational Mode of the molecule of water
2. How many peaks do we expect in the
    a. IR Spectrum
    b. Raman Spectrum
3. Here you have the Raman and IR spectrum of the Acetylene (H-C≡C-H)
    a. Explain why we observed those peaks in both spectrum
    b. Try to find at what vibrational modes correspond the peaks in each spectrum

Answer in-class activity

1. H_2O molecule is a non-linear molecule due to the uneven distribution of the electron density. O_2 is more electronegative than H_2 and carries a negative charge, while H has a partial positive charge. The total degrees of freedom for H_2O will be

Q=3*3-6 = 3 degrees of freedom

which correspond to the following stretching and bending vibrations. The vibrational modes are illustrated below:



2. We will expect 3 peaks in both spectrum, because the 3 vibrational modes are IR and Raman actives

Answer in-class activity

- 3. No effect on the Stokes, but it would increase the intensity of the anti-stokes intensity. Because raising the temperature would increase the population of vibrationally excited molecules such that the intensity of the anti-Stokes lines will increase.

- 4. If we consider the molecule of Acetylene, we will have 7 normal vibrational modes. We have a linear molecule and 4 atoms.

$$Q=3*4-5=7$$

Answer in-class activity

C-H symmetric stretching
3476 cm^{-1}
(IR inactive)
(Raman active)

H-C-C-H wagging
929 cm^{-1}
(IR intensity = 0.37)
(Raman inactive)

C-H asymmetric stretching
3423 cm^{-1}
(IR intensity = 1.0)
(Raman inactive)

H-C-C-H wagging
929 cm^{-1}
(IR intensity = 0.37)
(Raman inactive)

C-C-H bending
805 cm^{-1}
(IR inactive)
(Raman active)

C-C stretching
2181 cm^{-1}
(IR inactive)
(Raman active)

C-C-H bending
805 cm^{-1}
(IR inactive)
(Raman active)