

IR Spectrum 16.02: Acetone

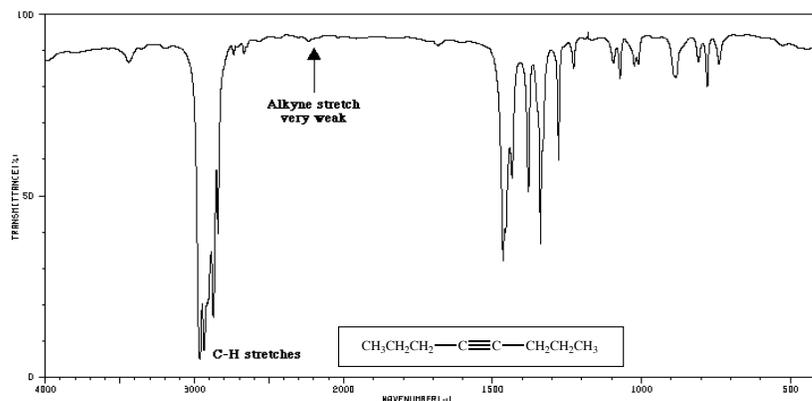
Answer: We are comparing two bonds, so we focus on their differences. Hooke's Law (section 16.04) tells us that differences in bond order (single versus double bond) or differences in the masses of the bonded atoms (C–H versus C–O) influence the stretching frequency, but it says nothing about the absorption intensity. So what other differences between the C–H and C=O bonds account for the intensity difference?

One difference worthy of exploration is the relative polarity of the two bonds. (You may want to review bond polarity from section 1.xx.) The electronegativity difference between carbon and hydrogen is small ($\Delta EN = 0.4$), whereas the electronegativity difference between carbon and oxygen is much larger ($\Delta EN = 1.0$). Therefore the C=O bond is more polar than the C–H bond. In the IR spectrum, the less polar C–H bond has smaller absorption intensity than the more polar C=O bond.

Studies of many IR spectra show this correlation to be broadly true. *In general, less polar bonds cause weaker absorptions (smaller peaks) than more polar bonds.* For example, the C–H bonds of 4-octyne (IR spectrum 16.03) are slightly polar whereas the C≡C bond is nonpolar (because it is symmetrical). In the IR spectrum, the sp^3 C–H stretches appear at 2963–2669 cm^{-1} whereas the C≡C stretch which usually occurs ~ 2200 cm^{-1} so weak that it cannot be seen.

Concept Connection

Bond polarity (1.xx)



IR Spectrum 16.03: IR spectrum of 4-octyne, illustrating the relative intensities of the sp^3 C–H and C≡C stretch peaks.

This same bond polarity effect causes the C=O stretch absorption to be more intense than most other peaks in the IR spectrum. Carbonyl stretches occur 1850–1650 cm^{-1} , a region of the IR spectrum that usually does not contain any other intense peaks. Therefore it is easy to decide if an unknown molecule has a carbonyl group. For example, in IR spectrum 16.04 the carbonyl stretch peak (1710 cm^{-1}) is strong.