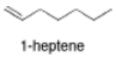
3.4: Carbon-Carbon Multiple Bonds

Unsaturated hydrocarbons contain only carbon and hydrogen, but also have some multiple bonds between carbons. One type of unsaturated hydrocarbon is an olefin, also known as an alkene. Alkenes contain double bonds between carbons. One example of an alkene is 1-heptene. It looks similar to hexane, except for the double bond from the first carbon to the second.



1-heptene

Look at the IR spectrum of 1-heptene. You should see:

- a set of peaks dipping down from the baseline at about 2900 cm^{-1}.
- another set of peaks dipping down from the baseline at about 1500 cm^{-1}.

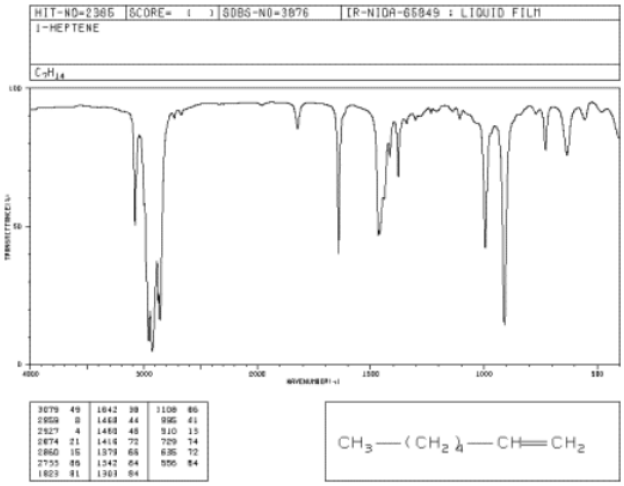


Figure 3.4.1: IR spectrum of 1-heptene.

So far, these peaks are the same as the ones seen for hexane. We can assign them as the C-H stretching and bending frequencies, respectively.

Looking further, you will also see:

- a small peak around 3100 cm^{-1}.
- a small peak near 1650 cm^{-1}.
- medium peaks near 900 and 1000 cm^{-1}.

The peak at 3100 cm^{-1} hardly seems different from the C-H stretch seen before. It is also a C-H stretch, but from a different type of carbon. This stretch involves the sp^2 or trigonal planar carbon of the double bond, whereas the peak at 2900 involves an sp^3 or tetrahedral carbon.

The peak at 1650 cm^{-1} can be identified via computational methods as arising from a carbon-carbon double bond stretch. It is a weak stretch because this bond is not very polar. Sometimes it is obscured by other, larger peaks.

The larger peaks near 800 and 1000 cm^{-1} are bending vibrations. They are due to a C=C-H bond angle that bends **o**ut **o**f the **p**lane of the double bond (remember that the carbons on either end of the double bond are trigonal planar). They are called oop bends. Oop bends are often prominent in alkenes and are easier to spot than an sp^2 C-H stretching mode or a C=C stretching mode.

? Exercise 3.4.1

Given this information about the infrared spectra of alkenes, which bond do you think is stronger, an sp^2 or an sp^3 C-H bond?

Answer

A $C_{sp}2$-H bond is stronger than a $C_{sp}3$-H bond.

Exercise 3.4.2

What do you think would happen to the peak due to carbon-carbon double bond stretching if an electronegative atom were nearby in the molecule?

Answer

The electronegative atom would polarize the nearby C=C bond. The C=C peak in the IR spectrum would become more intense; it might be a medium-sized peak instead of a weak one.

Exercise 3.4.3

Oop bends can be diagnostic of the position and geometry of double bonds.

a. Compare the oop bending modes or peaks seen in 1-heptene to those in *Z*-2-octene, aka *cis*-2-octene (in *Z*-2-octene, the double bond adopts a curled shape with alkyl substituents coming from the same side of the double bond).

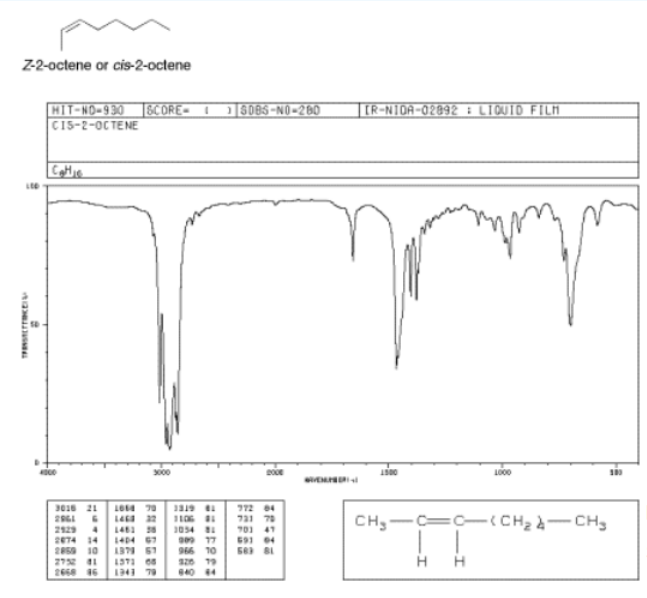


Figure 3.4.2: IR spectrum of Z-2-octene. Source: SDBSWeb : http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology of Japan, 14 July 2008)

b. Also compare it to *E*-2-octene, aka trans-2-octene (in which the double bond has a zig-zag shape, with alkyl substituents coming from opposite sides).

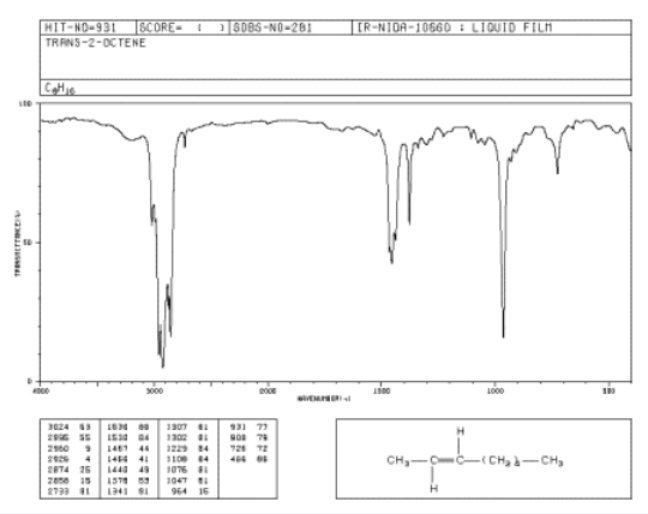
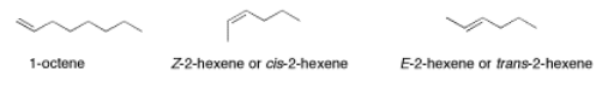


Figure 3.4.3: IR spectrum of *E*-2octene.

Source: SDBSWeb : http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology of Japan, 14 July 2008)

c) Make predictions about the oop bending modes in 1-octene, *Z*-2-hexene and *E*-2-hexene.



Answer

a) In the terminal alkene, in which the double bond was at the end of the chain, there were two oop bends showing at 900 and 1000 cm^{-1}. In the internal, *cis*-alkene, a single oop bend shows near 700 cm^{-1}.

b) In the *cis*-alkene, a single oop bend shows near 700 cm^{-1}. In the *trans*-alkene, that single oop bend shifts closer to 1000 cm^{-1}.

c) 1-octene: two IR bands, near 900 and 1000 cm^{-1}.

cis-2-hexene: one IR bands, near 700 cm^{-1}.

trans-2-hexene: one IR band, near 1000 cm^{-1}.

? Exercise 3.4.4

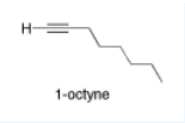
Why do you think an sp^3 CH_2 bending mode occurs around 1500 cm^{-1} but a C=CH oop bending mode occurs around 800-1000 cm^{-1} ?

Answer

A CH_2 or H-C-H bending mode involves three atoms: two hydrogens and a carbon. A C=C-H oop bend also involves three atoms: two carbons and a hydrogen. The reduced mass of the atoms involved in the oop bend is greater than the reduced mass of the atoms involved in the CH_2 bend. The oop bend shows up at a lower frequency.

? Exercise 3.4.5

In the IR spectrum of 1-octyne, new peaks appear at 3300 and 2100 cm^{-1}.



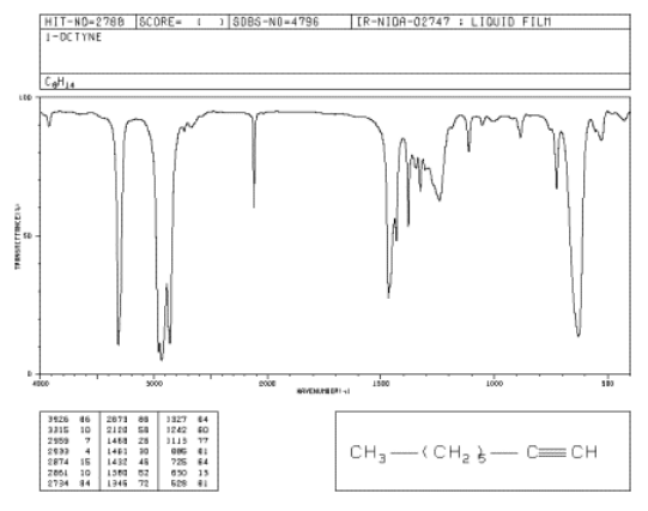


Figure 3.4.4: IR spectrum of octyne.

Source: SDBSWeb : http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology of Japan, 14 July 2008)

a. By comparison with the other hydrocarbons, can you identify the peak at 3300 cm^{-1} ?
b. The peak at 2100 cm^{-1} is due to a carbon-carbon bond. Which one? Compare this peak to the one seen from a carbon-carbon bond in 1-hexene and explain the differences.

This page titled 3.4: Carbon-Carbon Multiple Bonds is shared under a CC BY-NC 3.0 license and was authored, remixed, and/or curated by Chris Schaller via source content that was edited to the style and standards of the LibreTexts platform.