

3.3: Some Subtle Points of IR Spectroscopy

Alkanes show two sets of peaks in the IR spectrum. Alkanes contain two kinds of bonds: C-C bonds and C-H bonds. However, these two facts are not related. The reasons are explained through bond polarity and molecular vibrations.

Bond polarity can play a role in IR spectroscopy.

- nature rules that only bonds that contain dipoles can absorb infrared light.
- C-C bonds are usually nonpolar and usually do not show up as peaks in the IR spectrum.
- C-H bonds are not very polar and do not give rise to strong peaks in the IR spectrum.
- a whole lot of small C-H peaks can add up together to look like one big peak. This would happen if a molecule contained many C-H bonds (a common situation).

Molecular vibrations play a major role in IR spectroscopy.

- IR light interacts with vibrating bonds. When light is absorbed, the bond has a little more energy and vibrates at a higher frequency.
- a bond does not have an exact, fixed length; it can stretch and compress. This is called a bond stretching vibration.
- Stretching C-H bonds in alkanes absorb light at around 2900 cm^{-1} .
- bond angles can also bend; for instance, the H-C-H bond angle can compress and stretch. This is called a bending vibration.
- Bending H-C-H angles in alkanes absorb light at around 1500 cm^{-1} .

The factors that govern what bonds (and what vibrations) show up at what frequencies are easily handled by computational chemistry software. In fact, prediction of absorption frequencies in IR spectra can be done using 17th century classical mechanics, specifically Hooke's Law (devised to explain the vibrational frequencies of springs). Computation is not the focus of this chapter but it may help you keep track of what kinds of vibrations absorb at what frequencies.

Hooke's Law states:

- the vibrational frequency is proportional to the strength of the spring; the stronger the spring, the higher the frequency.
- the vibrational frequency is inversely proportional to the masses at the ends of the spring; the lighter the weights, the higher the frequency.

IR light is absorbed if it is in resonance with a vibrating bond; that means the light's frequency is the same as the frequency of the bond vibration, or else an exact multiple of it (2x, 3x, 4x...). It's a little like pushing a child on a swing: unless you are pushing at the same frequency that the swing is swinging, you will not be able to transfer your energy to the swing.

Hooke's Law in IR spectroscopy means:

- stronger bonds absorb at higher frequencies.
- weaker bonds absorb at lower frequencies.
- bonds between lighter atoms absorb at higher frequencies.
- bonds between heavier atoms absorb at lower frequencies.

Remember, there are two factors here, so you won't be able to make predictions knowing only one factor. Some strong bonds may not absorb at high frequency because they are between heavy atoms. The information is presented mostly to help you organize what bonds absorb at what general frequencies after you have learned about them.

The reasons explaining why C-H bending vibrations are at lower frequency than C-H stretching vibrations are also related to Hooke's Law. An H-C-H bending vibration involves three atoms, not just two, so the mass involved is greater than in a C-H stretch. That means lower frequency. Also, it turns out that the "stiffness" of a bond angle (analogous to the strength of a spring) is less than the "stiffness" of a bond length; the angle has a little more latitude to change than does the length. Both factors lead to a lower bending frequency.

? Exercise 3.3.1

For each of the following pairs, identify which bond would show up at a higher wavenumber in the IR spectrum:

- a) C-H or C-O b) C-O or C=O c) C=N or C≡N
d) N-H or N-O e) a covalent O-H bond or a hydrogen bond in water

Answer

- a) C-H shows up at higher wavenumber, because H is lighter than O
- b) C=O shows up at higher wavenumber, because a double bond is stronger than a single
- c) C=N shows up at higher wavenumber, because a triple bond is stronger than a double
- d) N-H shows up at higher wavenumber, because H is lighter than O
- e) Covalent O-H shows up at higher wavenumber, because a covalent bond is stronger than a hydrogen bond

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