

### 3.6: Carbon-Oxygen Double Bonds

The largest class of oxygen-containing molecules is carbonyl compounds, which contain C=O bonds. A C=O stretch is normally easy to find in an IR spectrum, because it is very strong and shows up in a part of the spectrum that isn't cluttered with other peaks. Examples of carbonyl compounds include 2-octanone, a ketone, and butanal, an aldehyde. In an aldehyde, the carbonyl is at the end of a chain, with a hydrogen attached to the carbonyl carbon.



If you look at the IR spectrum of 2-octanone:

- there are  $\text{sp}^3$  C-H stretching and  $\text{CH}_2$  bending modes at  $2900$  and  $1500\text{ cm}^{-1}$ .
- there is a very strong peak around  $1700\text{ cm}^{-1}$ .

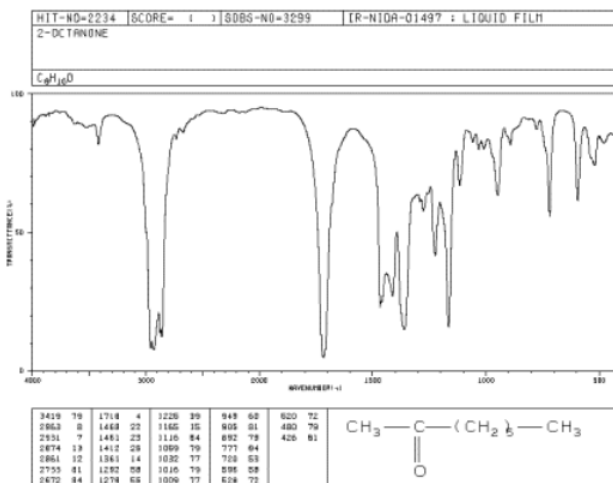


Figure 3.6.1: IR spectrum of 2-octanone.

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

Even though there is just one C=O bond, the carbonyl stretch is often the strongest peak in the spectrum. That makes carbonyl compounds easy to identify by IR spectroscopy.

If you look at the IR spectrum of butanal:

- there are  $\text{sp}^3$  C-H stretching and  $\text{CH}_2$  bending modes at  $2900$  and  $1500\text{ cm}^{-1}$ .
- there is a very strong C=O peak around  $1700\text{ cm}^{-1}$ .
- there is a pair of medium peaks around  $2700$  and  $2800\text{ cm}^{-1}$ . This is the aldehyde C-H stretching mode.

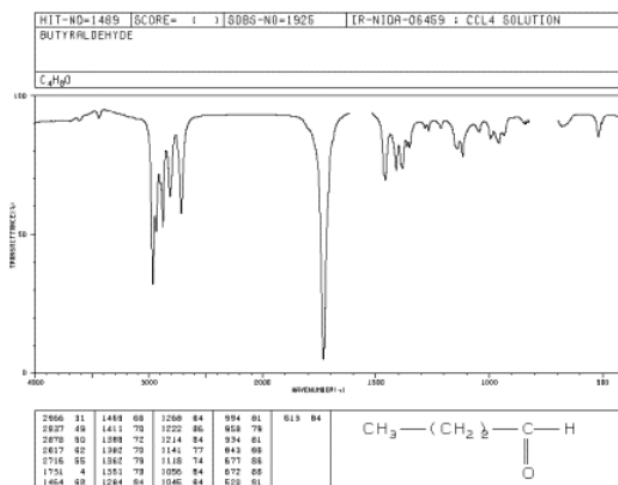


Figure 3.6.2: IR spectrum of butanal.

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

The aldehyde C-H bond absorbs at two frequencies because it can vibrate in phase with the C=O bond (a symmetric stretch) and out of phase with the C=O bond (an asymmetric stretch), and these vibrations are of different energies. The probability of the symmetric stretch and the asymmetric stretch are about equal, so the two peaks are always about the same size. This unusual C-H peak can often be used to distinguish between an aldehyde and a ketone.

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