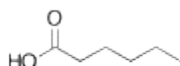


## MORE COMPLICATED SPECTRA

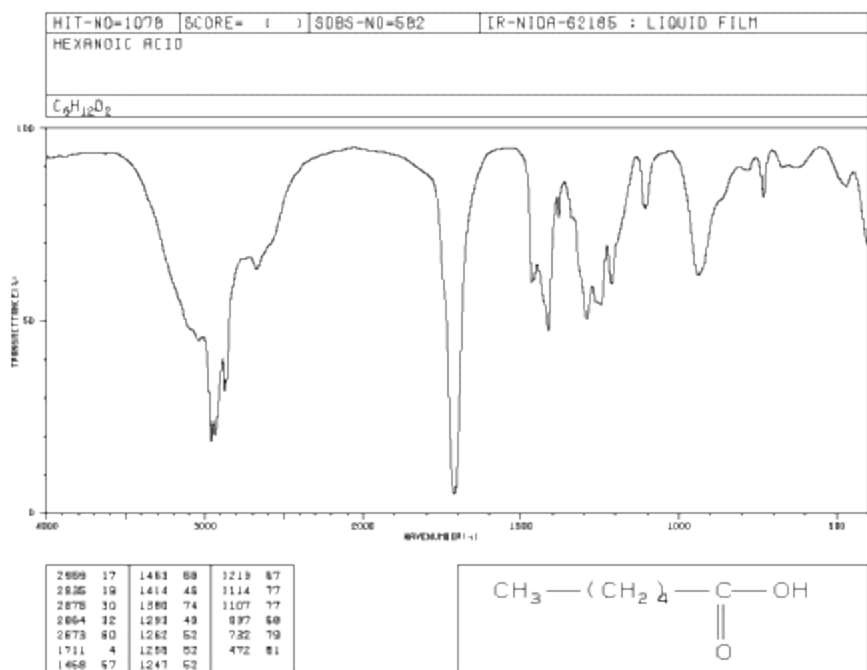
Sometimes more complicated heteroatomic functional groups, containing bonds to more than one heteroatom, have slightly different spectra. Carboxylic acids feature a hydroxyl group bonded to a carbonyl. Hexanoic acid, a carboxylic acid in a six-atom chain, is one example.



hexanoic acid

If you look at the IR spectrum of hexanoic acid:

- there are CH<sub>2</sub> bending modes at 1500 cm<sup>-1</sup>.
- there is a very strong C=O peak around 1700 cm<sup>-1</sup>.
- there is a medium C-O peak around 1250 cm<sup>-1</sup>.
- the sp<sup>3</sup> C-H and O-H stretching modes are less clear.



**Figure IR8.1.** IR spectrum of hexanoic acid.

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

At first, the O-H peak appears to be absent. The C-H stretch appears to be very broad. The wide peak between 3000 and 2600 cm<sup>-1</sup> is really the usual C-H stretch with a broad O-H stretch superimposed on it. The low frequency vibration of this O-H bond is related to the partial dissociation of protons due to strong hydrogen bonding.

Source : <http://employees.csbsju.edu/cschaller/Principles%20Chem/structure%20determination/IRComplicated.htm>