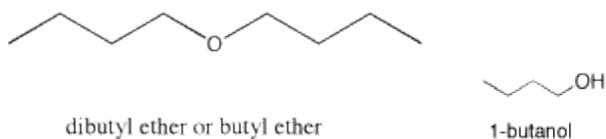


# BONDS TO COMMON HETEROATOMS: OXYGEN

These bonds are pretty polar, so they show up strongly in IR spectroscopy. IR spectroscopy is therefore a good way to determine what heteroatom-containing functional groups are present in a molecule.

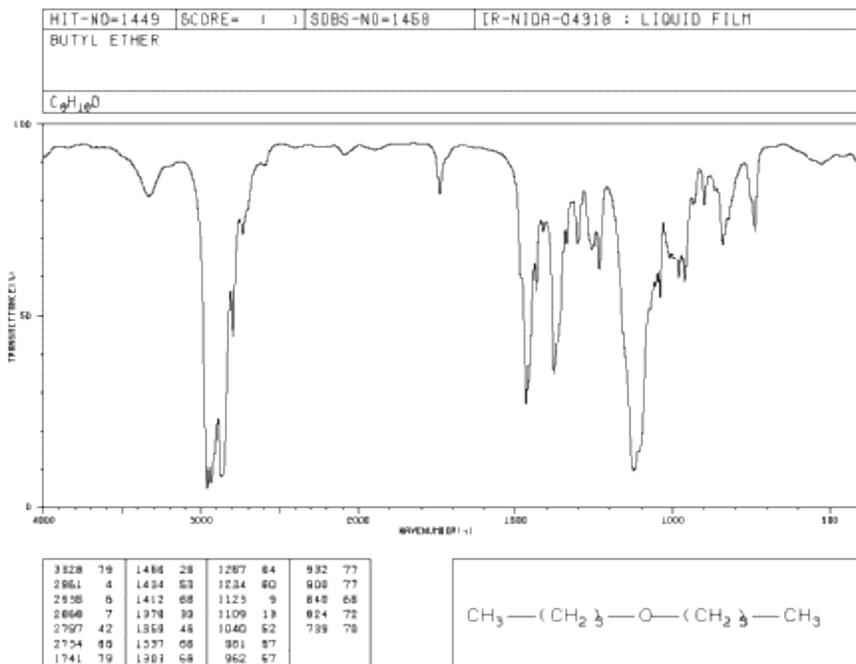
## Compounds Containing C-O Single Bonds

Oxygen forms two bonds. An oxygen atom could be found in between two carbons, as in dibutyl ether, or between a carbon and a hydrogen as in 1-butanol. Dibutyl ether is an example of an ether and 1-butanol is an example of an alcohol.



If you look at an IR spectrum of dibutyl ether, you will see:

- there are the usual  $sp^3$  C-H stretching and  $CH_2$  bending modes at  $2900$  and  $1500\text{ cm}^{-1}$ .
- there is a strong peak near  $1000\text{ cm}^{-1}$ . This peak is due to the C-O stretching vibration.

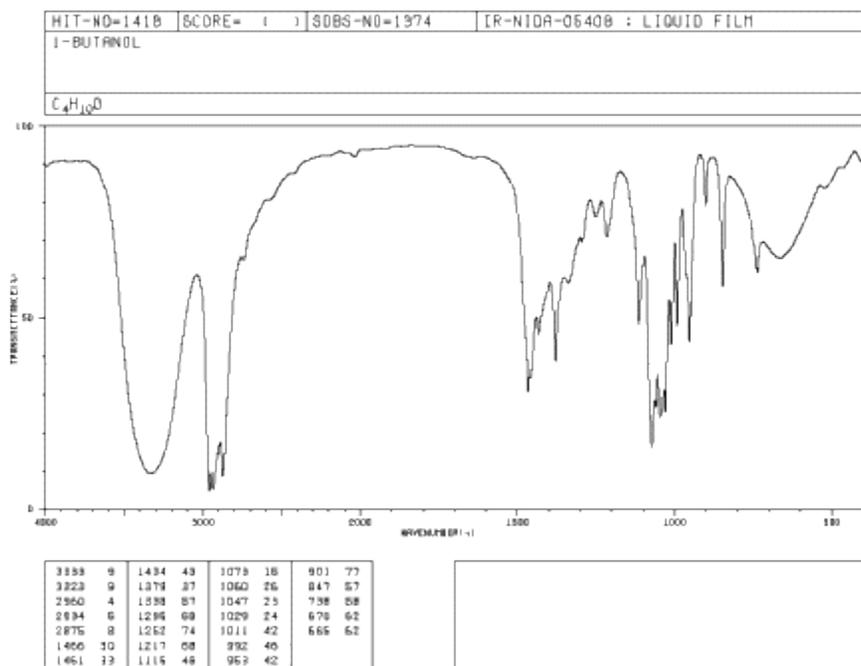


**Figure IR5.1.** IR spectrum of dibutyl ether.

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

If you look at an IR spectrum of 1-butanol, you will see:

- there are  $sp^3$  C-H stretching and  $CH_2$  bending modes at 2900 and 1500  $cm^{-1}$ .
- there is a strong C-O stretching mode near 1000  $cm^{-1}$ .
- there is a very large peak around 3400  $cm^{-1}$ . O-H peaks are usually very broad like this one.



**Figure IR5.2.** IR spectrum of 1-butanol.

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

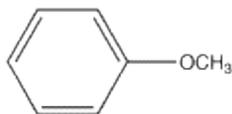
Peak shapes are sometimes very useful in recognizing what kind of bond is present. The rounded shape of most O-H stretching modes occurs because of hydrogen bonding between different hydroxy groups. Because protons are shared to varying extent with neighboring oxygens, the covalent O-H bonds in a sample of alcohol all vibrate at slightly different frequencies and show up at slightly different positions in the IR spectrum. Instead of seeing one sharp peak, you see a whole lot of them all smeared out into one broad blob. Since C-H bonds don't hydrogen bond very well, you don't see that phenomenon in an ether, and an O-H peak is very easy to distinguish in the IR spectrum.

#### Problem IR5.1.

Even though there are only two C-O bonds in dibutyl ether, the C-O stretching mode is even stronger than the peak at 2900  $cm^{-1}$  arising from 10 different C-H bonds. Explain why.

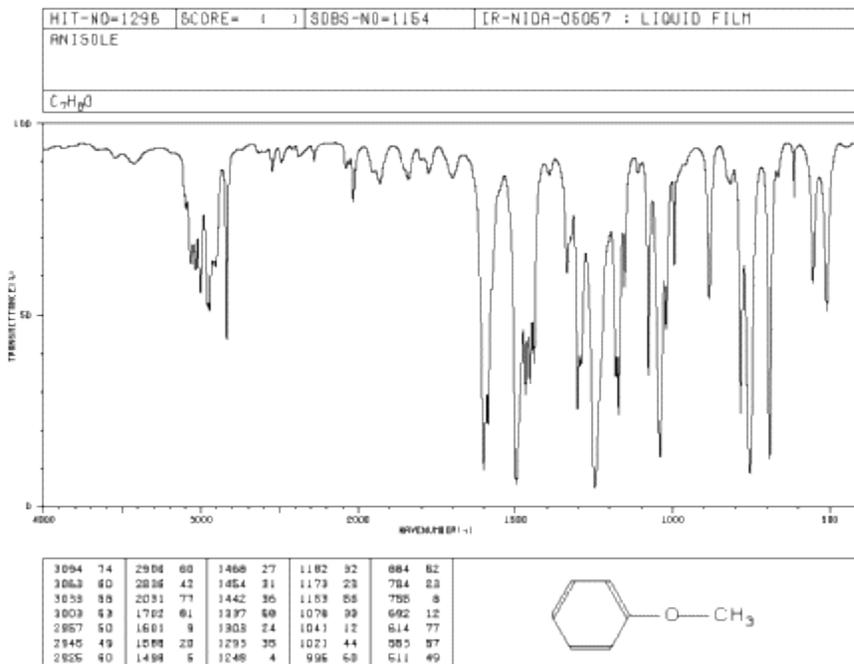
## Problem IR5.2.

The IR spectrum of methyl phenyl ether (aka anisole) has strong peaks at 1050 and 1250  $\text{cm}^{-1}$ .



methoxybenzene

- Identify the type of bond corresponding to these two peaks.
- Why are there two peaks for this type of bond in this molecule, and not just one?
- Draw a second, zwitterionic resonance structure for methyl phenyl ether.
- Use the zwitterionic resonance structure to explain why one of these bonds shows up at a higher frequency than the other one.



**Figure IR5.3.** IR spectrum of methyl phenyl ether.

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

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