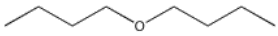
15.2: SPECTROSCOPY OF ETHERS

INFRARED SPECTROSCOPY

Oxygen forms two bonds. An oxygen atom could be found in between two carbons, as in dibutyl ether.



dibutyl ether or butyl ether

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 cm^{-1}.
- there is a strong peak near 1000 cm^{-1}. This peak is due to the C-O stretching vibration.

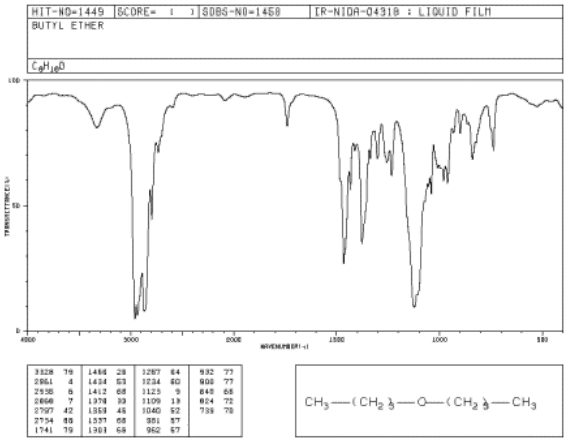
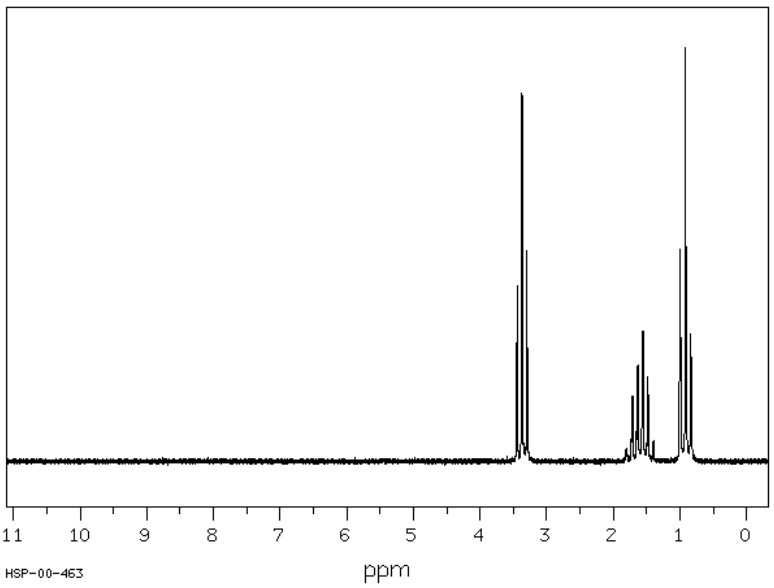


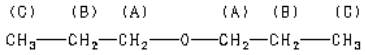
Figure IR. IR spectrum of dibutyl ether. Source: SDBSWeb: http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology of Japan, 14 July 2008)

NMR SPECTROSCOPY

- Hydrogens on carbon adjacent to the ether show up in the region of 3.4-4.5 ppm.
- Similar peaks in epoxides are shifted to a slightly higher field than other ethers. Hydrogens on carbons in and epoxide show up at 2.5 to 3.5 ppm.

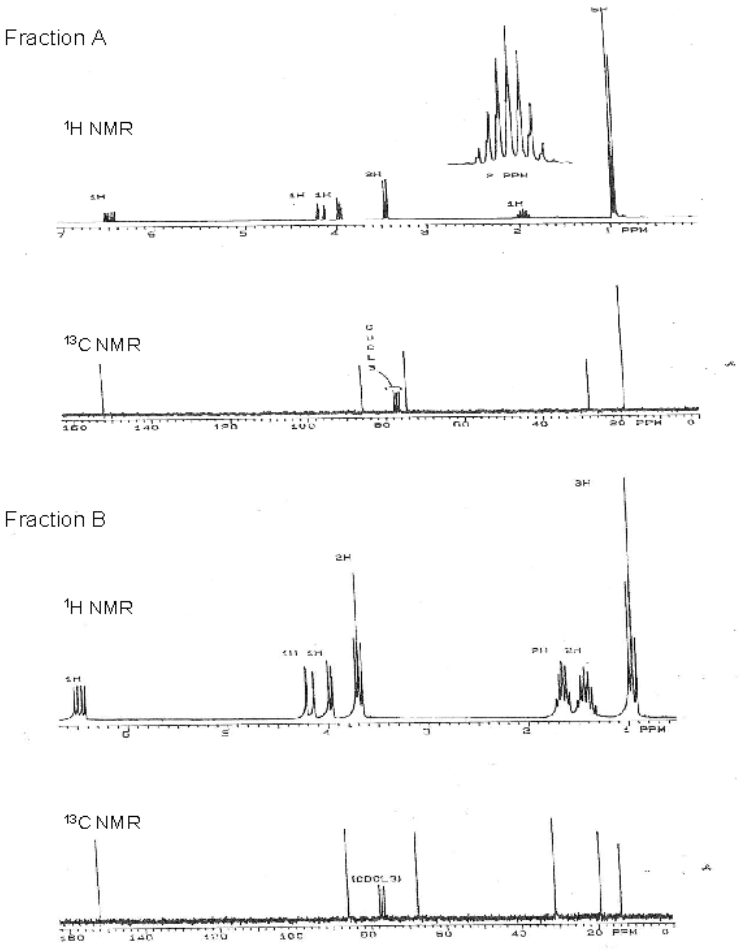
The 1H NMR spectrum of dipropyl ether shows three signals with the triplet at 3.37 ppm assigned to the -CH_2- beside the ether and the other two signals upfield (1.59 and 0.93 ppm). Notice the protons closer to the electron withdrawing oxygen atom are further downfield indicating some deshielding. Protons at (A) and (C) are each coupled to two equivalent (B) protons. So, each of these signals appears as a triplet. The (B) protons in turn are coupled to a set of two and three equivalent protons and you would therefore formally expect a quartet of triplets. However, because the coupling constants are very similar, the signal appears as a sextet. Source: SDBSWeb : http://sdbs.db.aist.go.jp (National Institute of Advanced Industrial Science and Technology, 28 June 2017)





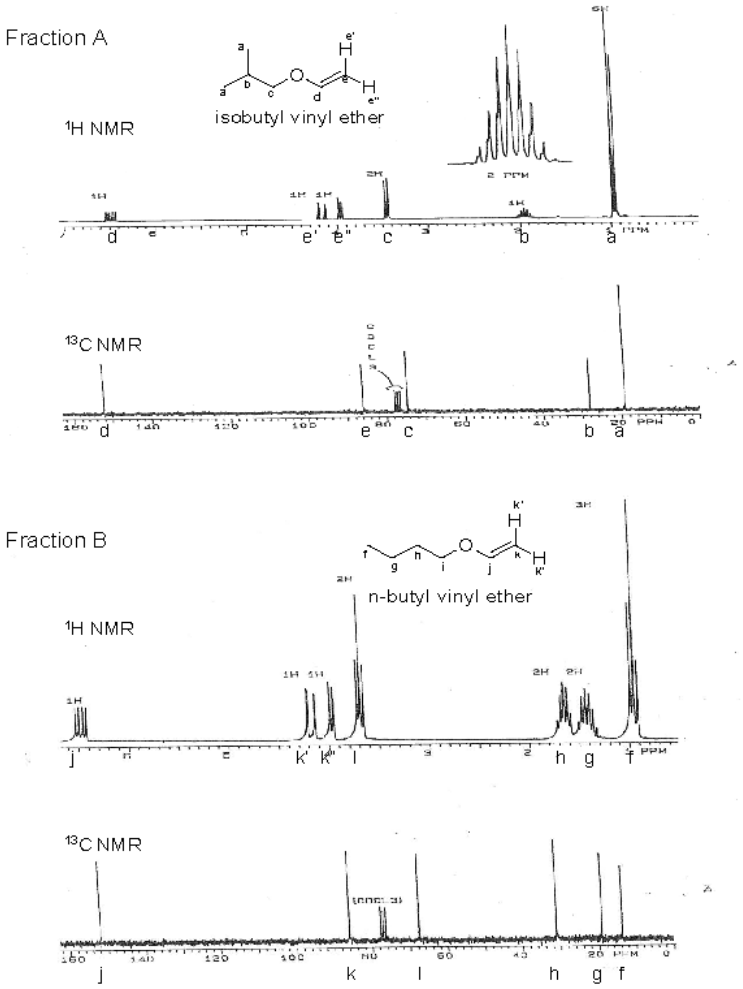
Exercise

2. A mixture of ethers was separated into two fractions: A and B. Elemental analysis reveals that the fractions are structural isomers: 72% C, 12% H, and 16% O. The IR spectra for both fractions show a couple weak bands near 3050 cm^{-1}, several stronger bands around 2950 cm^{-1}, and a strong, sharp band near 1204 cm^{-1}. The proton and ^{13}C NMR spectra for each fraction are shown below. Give the common name and draw the bond-line structure for each fraction and correlate the NMR signals with their respective atoms.



Answer

2.



CONTRIBUTORS AND ATTRIBUTIONS

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