

PROBLEM-SOLVING STRATEGY

Interpreting Proton NMR Spectra

Learning to interpret NMR spectra requires practice with a large number of examples and problems. The problems at the end of this chapter should help you gain confidence in your ability to assemble a structure from the NMR spectrum combined with other information. This section provides some hints that can help make spectral analysis a little easier.

When you first look at a spectrum, consider the major features before getting bogged down in the minor details. Here are a few major characteristics you might watch for:

- 1. If the molecular formula is known, use it to determine the number of elements of unsaturation (see Section 7-3). The elements of unsaturation suggest rings, double bonds, or triple bonds. Matching the integrated peak areas with the number of protons in the formula gives the numbers of protons represented by the individual peaks.
- Any broadened singlets in the spectrum might be due to —OH or —NH protons. If the broad singlet is deshielded past 10 ppm, an acid —OH group is likely.

3. A signal around δ3 to δ4 suggests protons on a carbon bearing an electronegative element such as oxygen or a halogen. Protons that are more distant from the electronegative atom will be less strongly deshielded.

$$-0 C-H$$
 $Br-C-H$
 $Cl-C-H$
 $I-C-H$

around $\delta 3 - \delta 4$ for hydrogens on carbons bearing oxygen or halogen

4. Signals around $\delta 7$ to $\delta 8$ suggest the presence of an aromatic ring. If some of the aromatic absorptions are farther downfield than $\delta 7.2$, an electron-withdrawing substituent may be attached.