

The distance between individual lines in a signal is called the **coupling constant** (or J value). Spin-spin splitting is not dependent on the external field, so we use energy units for coupling constants (Hz).

In the ^1H NMR spectrum of 2-pentanone, due to their integration of 3 we were able to assign the signals at $\delta = 0.93$ ppm and $\delta = 2.10$ ppm to the methyl groups. The signal at $\delta = 2.10$ ppm is singlet, while the signal at $\delta = 0.93$ appears as a triplet. When we count the distance between the protons of the each methyl group and its closest non-equivalent neighboring protons, we note that the protons bound to the methyl group adjacent to the carbonyl group have no nonequivalent protons within its three bonds. In contrast, the protons of the other methyl group are within three bonds of a methylene group. Thus, these methyl protons are able to "see" the spin state of each of the methylene protons and their signal is split into $n+1$ lines. With $n = 2$, those methyl protons "see" two non-equivalent protons and their signal is split into a triplet. Thus the signal at $\delta = 2.10$ ppm – a singlet – is due the methyl protons adjacent to the carbonyl group, while the signal at $\delta = 0.93$ ppm – a triplet – is due to the methyl protons further away from the carbonyl group. We can repeat this with the signals for the methylene groups in this molecule and determine that the signal at 2.40 ppm – a triplet with an integration of 2 – is due to the methylene group adjacent to the carbonyl group. Its protons are three bonds from the two nonequivalent protons of the other methylene group. Thus with $n = 2$ this signal is expected to be a triplet. The remaining methylene group signal at $\delta = 1.60$ ppm is a sextet due its proximity to the methyl group, and the methylene group adjacent to the carbonyl group (Figure 9.6).



FIGURE 9.6. Signal splitting in the ^1H NMR spectra of isomeric pentanones.

The signal at $\delta = 2.45$ ppm, which we already assigned as being the methylene group in 3-pentanone, appears as a quartet. The signal at $\delta = 1.06$ ppm – the methyl protons – appears as a triplet. This triplet/quartet coupling pattern with a ratio of integration of 3:2 is very characteristic of ethyl groups.

Typical splitting patterns for common alkyl groups and substituted benzenes are summarized in Table 9.2 and Table 9.3, respectively.

TABLE 9.2. Splitting pattern of some alkyl groups R-X.

R-X	NUMBER OF SIGNALS	SPLITTING PATTERN/ INTEGRATION
Methyl: $\text{CH}_3\text{-X}$	1	One singlet
Ethyl: $\text{CH}_3\text{CH}_2\text{-X}$	2	One 2H quartet One 3H triplet
Propyl: $\text{CH}_3\text{CH}_2\text{CH}_2\text{-X}$	3	One 2H triplet One 3H triplet One 2H sextet
Isopropyl: $(\text{CH}_3)_2\text{CH-X}$	2	One 6H doublet One 1H septet
Butyl: $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{-X}$	4	One 2H triplet One 3H triplet One 2H quintet One 2H sextet
tert-Butyl: $(\text{CH}_3)_3\text{C-X}$	1	One singlet

TABLE 9.3. Splitting pattern of benzene and substituted aromatic compounds.

	NUMBER OF SIGNALS	SPLITTING PATTERN/ INTEGRATION
	1	One singlet
	3	One 2H doublet One 2H triplet One 1H triplet
	2	One 2H doublet One 2H triplet
	3	One 1H singlet One 2H doublet One 1H triplet
	1	One singlet
	4	Two 1H doublets Two 1H triplets