13C NMR Number of Signals

Transcript

00:00:01:80 - 00:00:10:18
Dr.Jessie Key: Hello again, Dr. Jessie Key here. In this video, examine chemical equivalents and number of signals in carbon NMR.

00:00:10:18 - 00:00:28:94
Dr.Jessie Key: A few examples of common alkyl and aromatic patterns will also be examined. Carbons which can be related by rotational symmetry are considered chemically equivalent and will appear as the same signal. Let's take a look at a simple example, propane, C3H8.

00:00:28:94 - 00:00:58:19
Dr.Jessie Key: The 3-D ball and stick diagram provided shows the carbons of propane in gray and the hydrogens in white. If we rotate the molecule 180 degrees, notice that carbons 1 and 3 swap positions, This is an example of rotational symmetry relating these two carbons, making them chemically equivalent. Therefore, propane will have two signals total in its carbon NMR. A signal for carbon 2,

00:00:58:19 - 00:01:19:48
Dr.Jessie Key: and a signal for carbons 1 and 3. Carbons which are seen to be symmetrically related by a plane of reflection are also considered chemically equivalent and will appear as the same signal. Let's take a look at another simple example, isopropanol, C3H8O.

00:01:19:92 - 00:01:43:30
Dr.Jessie Key: Again, the 3-D ball and stick diagram provided shows the carbons in gray, the hydrogens in white, and the oxygen in red. This diagram makes it easy to see there's a mirror plane running down the center of the molecule, relating the two methyl carbons by a plane of reflection. They are therefore chemically equivalent and will show up as one signal.

00:01:43:30 - 00:01:59:64
Dr.Jessie Key: A second signal would be observed for the central carbon. Therefore, a total of two signals is expected for isopropanol. In this slide, we'll examine the number of signals we would expect to find for some of the more common 3- and 4- carbon branched alkanes.

00:01:59:64 - 00:02:21:84
Dr.Jessie Key: Pattern recognition can help in the rapid interpretation of NMR spectra. Starting with the three carbon patterns: propyl groups have no symmetry relating the carbons, so we would see three signals, one for each carbon. Isopropyl methyls are chemically equivalent by symmetry, and therefore, we would expect to see two signals.

00:02:21:84 - 00:02:44:29
Dr.Jessie Key: For the four carbon branched alkanes, we see four signals expected for both butyl and sec-butyl since there is no symmetry relating any of the carbons. Isobutyl would display three signals as the two methyl carbons are related by symmetry. Finally, tert-butyl has all three of its methyl groups related by symmetry.

00:02:44:29 - 00:03:00:85
Dr.Jessie Key: So only two signals are expected. The substitution patterns of aromatic rings affect the number of carbon 13C signals. On this slide, we have three constitutional isomers of the molecule dimethyl benzene, commonly called xylene which we'll examine.

00:03:00:85 - 00:03:27:94
Dr.Jessie Key: The 1, 4- dimethyl isomer produces three signals, as there are two symmetry planes shown as dash red lines running vertically and horizontally through the structure. This makes all four ring carbons highlighted in brown chemically equivalent. The two ring carbons at the 1- and 4- positions are related by the horizontal plane of symmetry, and the two methyl carbons are also similarly related.

00:03:27:94 - 00:03:46:36
Dr.Jessie Key: The 1,2-dimethyl isomer produces four signals. There's a single plane of symmetry, which is shown by the dash red line running horizontally through the structure. This relates each of the four carbons above with their reflected carbons below.

00:03:46:36 - 00:04:06:60
Dr.Jessie Key: Finally, 1,3-dimethylbenzene produces five signals. Similarly, it has a single plane of symmetry, which is shown by the dash red line running vertically through the structure. This relates each of the three carbons to the left side of the plane with their reflected carbons on the right side of the plane.

00:04:06:60 - 00:04:15:54
Dr.Jessie Key: However, the two central most carbons with the plane running through them are not related by symmetry and would appear as separate signals.