Neighbour Method

Transcript

Instructor: Jessie Key

00:00:00:00 - 00:00:22:52
Instructor: Hello again, Doctor Jesse Key here. This video focuses on showing an alternative or supplementary method for determining chemical equivalents and therefore the number of signals. But first, let's determine the number of signals using the previously shown symmetry method using a simple example, one, two, four trimethyl cyclopentane.

00:00:22:52 - 00:00:49:07
Instructor: Take a moment and with a pen and paper, draw in the plane of reflection. The plane of reflection can be identified by drawing a straight line horizontally through the center of this molecule as drawn. This would give us a total of five signals in our carbon 13 NMR.

00:00:49:07- 00:01:01:13
Instructor: Hopefully, you found that plane of reflection easily. However, this may not always be the case for more complex structures. Also, I found that some of us struggle with recognizing symmetry more than others.

00:01:01:13 - 00:01:37:61
Instructor: An alternate or supplementary approach that can be used which doesn't rely on recognizing symmetry is called the neighbors method. This method is built on the concept that the chemical shift of a given carbon NMR signal is dependent on the electronic environment of that carbon or the carbons comprising that signal. If two carbons have the exact same neighbors, they will experience the exact same electronic effects from those same neighbors, making them chemically equivalent, which produces a single signal.

00:01:37:61 - 00:01:57:48
Instructor: If two carbons have different neighbors, they will experience different electronic effects and therefore give rise to different signals. Let's take a look at this neighbors method, again, using one, two, four trimethyl cyclopentane. The neighbor method really excels at comparing two given nuclei.

00:01:57:48 - 00:02:43:20
Instructor: Let's compare the carbon highlighted in blue and the carbon highlighted in red in my new drawing of the structure. For the carbon highlighted in blue, if we go around clockwise, a few positions, its neighbors are a CH with a CH three attached, a CH two, and then another CH with a CH three attached. For that carbon in blue, if we go around counterclockwise, its

neighbors are a CH with a CH three attached.

00:02:45:72 - 00:03:13:16
Instructor: Then another CH with the CH three attached. Then finally, that CH two. If we perform that same analysis for a carbon highlighted in red, again, starting off going clockwise, we get the CH with the CH three attached.

00:03:16:64 - 00:03:37:20
Instructor: Then it's another CH with CH three attached. Then after that, we have a CH two. Going around counterclockwise from that carbon highlighted in red, we first encounter a CH CH three.

00:03:40:28 - 00:04:16:54
Instructor: Then it's a CH two. Then finally, a CHCH three. Now looking at these two lists of neighbors, we can see that our list going clockwise for the carbon highlighted in blue perfectly matches the list going counterclockwise for our carbon and red.

00:04:18:98 - 00:04:53:12
Instructor: Similarly, the list for our carbon and blue going counterclockwise, perfectly matches the list going clockwise for our red carbon. These two carbons have the exact same sets of neighbors, they should feel the same electronic effects and be the same signal. Let's compare another set of carbons within the same molecule.

00:04:53:12 - 00:05:24:97
Instructor: This time, the carbons highlighted in green and black. For the carbon highlighted in green, if we go around clockwise, its first neighbor is a CH two. Its next neighbor is a CH CH three, then its next neighbor after that is another CH CH three.

00:05:26:93 - 00:06:13:15
Instructor: If we go around counterclockwise, its first neighbor is a CH two, after that, we have a CH CH three, and then another CHCH three. If we compare to that carbon highlighted in black, going around clockwise, its first neighbor is a CHCH three. Immediately, we can see this is different from either of the neighbor sets for our carbon highlighted in green.

00:06:13:15 - 00:06:35:53
Instructor: Neither of our clockwise or counterclockwise sets of neighbors started with a CHCH three. This means that these have different neighbors. Therefore, these two carbons are different electronic environments because they have different neighbors and will give rise to different signals.