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Neighbour Method

Transcript

00:00:00:00 - 00:00:11:78
Dr.Jessie Key: Hello again, Dr. Jessie Key here. This video focuses on showing an alternative, or supplementary method, for determining chemical equivalents and therefore the number of signals.

00:00:11:78 - 00:00:49:69
Dr.Jessie Key: But first, let's determine the number of signals using the previously shown symmetry method using a simple example, 1, 2, 4-trimethlycyclopentane: 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. Hopefully,

00:00:49:69 - 00:01:01:13
Dr.Jessie Key: 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
Dr.Jessie Key: An alternate or supplementary approach that can be used which doesn't rely on recognizing symmetry is called the ‘neighbours 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 - 00:02:05:60
Dr.Jessie Key: If two carbons have different neighbors, they will experience different electronic effects and therefore give rise to different signals! So let's take a look at this neighbors method, again, using 1,2,4-trimethylcyclopentane. The neighbor method really excels at comparing two given nuclei, so let's compare the carbon highlighted in blue and the carbon highlighted in red in my new drawing of the structure.

00:02:08:17 - 00:03:25:04

Dr.Jessie Key: For the carbon highlighted in blue, if we go around clockwise a few positions, its neighbours are a CH with a CH three attached (CHCH3), a CH two (CH2), and then another CH with a CH three attached (CHCH3). For that carbon in blue, if we go around counterclockwise, its neighbors are a CH with a CH three attached (CHCH3), then another CH with the CH three attached(CHCH3), then finally, that CH two (CH2). 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 (CHCH3), then it's another CH with CH three attached (CHCH3), then after that, we have a CH two (CH2).

00:03:25:04 - 00:04:16:54
Dr.Jessie Key: Going around counterclockwise from that carbon highlighted in red, we first encounter a CH CH three (CHCH3). then it's a CH two (CH2), then finally, a CHCH three (CHCH3). 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 - 00:04:57:44
Dr.Jessie Key: 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, so they should feel the same electronic effects and be the same signal. Let's compare another set of carbons within the same molecule, this time, the carbons highlighted in green and black.

00:05:00:81 - 00:06:03:89
Dr.Jessie Key: For the carbon highlighted in green, if we go around clockwise, its first neighbour is a CH two (CH2), its next neighbour is a CH CH three (CHCH3), and then its next neighbour after that is another CH CH three (CHCH3). If we go around counterclockwise, its first neighbour is a CH two (CH2), after that, we have a CH CH three (CHCH3), and then another CH CH three (CHCH3). If we compare to that carbon highlighted in black, going around clockwise, its first neighbour is a CHCH three (CHCH3).

00:06:04:29 - 00:06:25:01
Dr.Jessie Key: Immediately, we can see this is different from either of the neighbour sets for our carbon highlighted in green. Neither of our clockwise or counterclockwise sets of neighbors started with a CHCH three (CHCH3). This means that these have different neighbours.

00:06:26:57 - 00:06:35:53
Dr.Jessie Key: Therefore, these two carbons are different electronic environments because they have different neighbours and will give rise to different signals!