Using NMR to Predict Molecular Structure

Transcript

Instructor: Brett McCollum

00:00:00:00 - 00:00:44:91
Instructor: All right. Now we're going to try a slightly more challenging example for a nuclear magnetic resonance. We have our proton NMR spectrum, and we've also been given that the IR spectra only shows alkanes, so we know there's no interesting functional groups present, and we also have our molecular mass at 100 atomic mass units. Finally, one more piece of information we've been given about our spectrum is that these two sets of peaks are in a two to three ratio in terms of their integration. As before, first thing we want to do is build our table from which we'll organize the information that's captured within the spectrum.

00:00:44:91 - 00:01:28:61
Instructor: We have our positions or we could write the word signals, if you prefer that. We have A, B, and C. For the chemical shift, we see that signal A shows up slightly lower than 1 PPM at about 0.9. Hopefully, you now recognize that 0.9 is where we tend to find CH3 groups.

00:01:28:61 - 00:01:52:03
Instructor: That's a really good hint that that's what our signal is. Then we have B, which is showing up a little bit higher at about 1.2 PPM. And signal C, which is showing up yet a little bit higher. Almost halfway 1-2, so we're going to put down that that's about 1.5 PPM.

00:01:52:31 - 00:02:06:95
Instructor: 1.3 on this. That that will be okay. We've got our chemical shifts of 0.9, 1.2, 1.3 and 1.5 or so PPM.

00:02:06:95 - 00:02:34:83
Instructor: Then we need our integrations. Now, we know that this is a three to two in terms of A to B. We're going to write that down, three to two ratio, and C, C is a really weak signal. Unless we've been given the integration, we don't really have a good way to figure out what that is, so we don't know. We're just going to put question mark for now.

00:02:34:83 - 00:02:59:79
Instructor: Let's move on to our multiplicities. A is clearly a one to two to one triplet. B appears to be five peaks. Again, a multiplet that we would call a quintet. C is just a mess.

00:02:59:79 - 00:03:27:12
Instructor: A really weak signal. Lots of peaks. It's not clear, we're just going to write that it's a multiplet. This is the information that we have, but as we mentioned before, we know that there are no other functional groups present. We're dealing with an alkane of some sort that has an atomic mass, sorry, a molecular mass of 100 atomic mass units.

00:03:27:12 - 00:04:19:43
Instructor: Now there's different directions we could go at this point. We could start off with the fact that we know it's an alkane, so that means it has a formula of only carbons and hydrogens. Now, if it's an alkane and it's all single bonds, then the number of hydrogens are known in terms of the number of carbons as 2x plus 2. We could figure out what x is by building an appropriate formula to get to a mass of 100. 12 times the number of carbons plus 1, that's the mass of a hydrogen, times the number of hydrogens, should equal 100 atomic mass units.

00:04:19:43 - 00:05:23:48
Instructor: That's 12x plus another 2x, 14x should equal 100 minus 2, 98, x will equal 7, and we can double check that we've done this right, that 12 times 7 plus 14 and 2 more. That's 84 and 16, which is 100 as we expect. We now know our chemical formula is C7H, 2 times 7 is 14, plus 2 more, 16. We compare with the information that we have here, we see a proton integration of 3 to 2 plus something else. That really weak signal might be something like a CH group because again, there's nothing else going on here in the IR, just an alkane.

00:05:23:48 - 00:06:02:02
Instructor: If we think that this is a CH of an integration of one, we take one off of our 16, we're left with 15 hydrogens remaining in the molecule in a three to two ratio. Really, that's 5, 3 times. I'm going to say this is probably a nine and six. Nine to six is still a three to two ratio. 9 plus 6 is 15 plus 1 more is 16, and that adds up to the number of hydrogens in our molecule. All right.

00:06:02:02 - 00:06:37:58
Instructor: We've got our integration, we've got a chemical shift. Let's look at these for a moment. Get out your table again, where you're able to compare to see what position groups tend to show up in a proton nuclear magnetic resonance experiment. We know that 0.9 tends to match with the CH3 group, 1.2 suggests a CH2 group and 1.5 a CH group.

00:06:37:94 - 00:07:11:64
Instructor: Can we match that with our multiplicities? If A is going to be a CH3 group, there should be one more bond attached to that. It is showing up as a triplet. A triplet suggests that it has two neighboring protons, meaning it is next to a CH2 group. Let's look at B. B is a CH2 group.

00:07:11:72 - 00:07:36:52
Instructor: It needs two more bonds to complete the octet. And it's showing up as a quintet, quintet suggesting that it has four neighbors. That could be a CH2 and another CH2. It could be a CH3 and an H. We already know that there's a CH3 and a CH, present in our compound.

00:07:36:52 - 00:08:07:42
Instructor: Namely signals A and C. Then finally, signal C, the CH group, will need three bonds to complete the octet. It's showing up as a multiply. It has lots of neighbors. Well, looking at our choices here, the CH has to be bonded to something that is bonded to it.

00:08:07:58 - 00:08:47:19
Instructor: That might sound like a redundant statement, but it's really important because it means look at the other signals and find what is the CH bonded to. The CH is not bonded to a CH3. The only place where detecting a CH is here, bonded to a CH2 group. But if it was only one CH2 group, that would show up as a triplet. It needs to be bonded to something else, and there's nothing else in this compound, but we do know that in fact, A comprises of three CH3 groups to get an integration of nine.

00:08:47:19 - 00:09:27:58
Instructor: There's this three times. B is a CH2 group three times to show up as an integration of six. If there are three CH2 groups, that explains all three bonds attached to that CH carbon. Now we're able to fit our molecule together using all the pieces that we've assembled. We have in the middle a CH that is bonded to CH2s, and each of those CH2s are bonded to a CH3.

00:09:27:58 - 00:09:51:64
Instructor: Put that together, and we can say that we have a CH3 to a CH2 to a CH, that is to a CH2, CH3, and a CH2 to a CH3. We have a pentane that position three has an ethyl group off of it. The answer is 3-ethylpentane.