TRU
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Using IR to Predict Molecular Structure

Transcript

Instructor: Brett McCollum

00:00:00:28 - 00:01:01:31
Instructor: I'm going to let you in on a secret. This is my favorite part of the course, nuclear magnetic spectroscopy. What we're going to do is we're going to identify the unknown compound using only an NMR spectrum, a proton NMR spectrum, and we've being given the molecular mass of our compound. To do this, we're going to have to be able to interpret what these peaks are telling us in terms of the chemical shift, the splitting pattern, the integration, and then relate that to the molecular mass of our compound. When I tackle one of these problems, one of the first things I always do is to build a table that helps me organize my thinking, because what you're doing is you are detangling a whole bunch of information, pulling it out of that spectrum, and then those are like pieces to a puzzle, and you need to be able to fit them together.

00:01:01:31 - 00:01:49:11
Instructor: But if you don't organize your puzzle pieces effectively, it's going to be much more difficult to solve the puzzle. Let's build our table. First thing I do is I write out the positions on my spectrum. We're going to call the first peak, A and the second one, B. Then we have our chemical shift scale here, Delta, and we see that Peak A shows up just slightly higher than 1 PPM at about 1.2.

00:01:50:47 - 00:02:04:47
Instructor: B is showing up higher than three, but not quite four. It's around 3.7, 3.8. Let's put 3.8. Then next,

00:02:04:47 - 00:02:39:62
Instructor: we have our integration. Now, in some cases, you may need to actually sum up the heights of your peaks if they're sufficiently narrow using a ruler, you could add how many millimeters and that could give you an estimate for the ratio. In other cases, we use software to actually measure the area under the curve, the integration of these peaks. In this case, I'm going to give you what those integrations are. This one is six hydrogens in a ratio with one hydrogen.

00:02:39:62 - 00:03:11:30
Instructor: Now, that doesn't guarantee that it is six and one, rather the ratio is six to one. It could be six and one, 12, and two, and so on. Next, we want to identify the multiplicity of our signals. Because remember multiplicity tells us information about how many neighboring hydrogens there are for that group of equivalent hydrogens. Peak A is a doublet.

00:03:11:30 - 00:04:04:98
Instructor: And a doublet means that there is one neighboring proton that is causing this set of equivalent hydrogens to be split from a singlet into a doublet. In contrast, B, it's a little hard to see, but if you look this multiplet actually has seven peaks to it. We could just write multiple, but in this case, because I can see those peaks, I might actually put down that I think it is a septet. Okay. For it to have that splitting pattern, that would indicate that there are six neighboring protons for whatever is causing signal B.

00:04:04:98 - 00:04:31:86
Instructor: We're now ready to start figuring out how we fit this information together to propose possible chemical structures. Keep in mind, we do have our molecular mass and we're going to have to refer back to that as we fit the pieces together. Let's start with signal A. It is potentially six protons. It's either six or 12.

00:04:31:86 - 00:04:57:40
Instructor: Let's assume it's six at first. That could be three CH2 or more likely, I think it is two CH3 groups. We could have a CH3 that has a neighbor. How many neighbors does it have? It has a neighbor that has one proton on it.

00:04:57:40 - 00:05:25:88
Instructor: That's why it's being split into a doublet. There are two of that happening in our molecule, and they have to be identical, otherwise they would show up as separate signals. That's what A is. Now, A has to be split by this neighbor. Well, how many other protons are there, how many other environments are there in this molecule.

00:05:25:88 - 00:06:13:64
Instructor: There's only one other environment. We know that the proton splitting signal A has to be the protons in signal B or the single proton of signal B. We know that B which is a CH group. It needs to have three more bonds to satisfy the octet of the carbon. It if it's a septet, that is six neighbors, which would be a CH3 group and another CH3 group, and that matches our expectation of six protons in signal A.

00:06:13:64 - 00:06:38:96
Instructor: We now understand why signal B has been split into a septet because it has six neighbors, which are signal A. But there's one more bond left. What's there? There's no more protons in our spectrum. Let's look at our molecular mass.

00:06:39:40 - 00:07:26:85
Instructor: We recognize that if we have one, two, three carbons present, each carbon has a mass of approximately 12 atomic mass units, and we are seeing seven protons in our signal.

That's 36 and seven more, that's 43 atomic mass units. If we take our total mass of 78.5 and we subtract the mass that we've now assigned within the spectrum, we are left with the mass of 35.5 atomic mass units.

00:07:26:85 - 00:08:03:74
Instructor: That, if you check your periodic table, matches the mass of what element? A single atom of chlorine. That might be what's on the end here. Before we go further, we've not yet thought about our chemical shift and whether or not we can explain why it's occurring. A CH3 group would normally show up, where in our chemical shift along that axis.

00:08:03:74 - 00:08:29:37
Instructor: Pause the video, get out your spectroscopy data sheet and check. Okay. We recognize that a CH3 group should generally show up if it's attached to another CL group, should show up around 0.9 PPM. It's been shifted a little bit higher to about 1.2 PPM,

00:08:29:37 - 00:09:06:68
Instructor: which suggests that we have something here that is not directly attached, but is one more bond away that is an electron withdrawing group. Something that is causing this set of protons to be slightly deshielded, shifting it down field to 1.2. In contrast, the CH3 group is directly attached to whatever that is, we think it's a chlorine atom, and it is significantly deshielded. If we check our data sheet, we think this is a chlorine.

00:09:06:68 - 00:09:29:19
Instructor: What is the range in a proton NMR spectrum where you expect a proton to show up when it is attached to a carbon right next to a chlorine group? Check your data sheet now. Hopefully, you agree with me, it should be around 3.1 to 3.8 PPM.

00:09:29:19 - 00:09:49:55
Instructor: Recognizing that the low end of that spectrum is for a CH3 group. The mid range is for a CH2 and the high range of that is going to be for a CH. We expect this CH group to show up around 3.8 PPM. Where did we say it shows up?

00:09:49:55 - 00:10:16:52
Instructor: 3.8. Exactly, where our data sheet would expect. This is awesome that we're able to see these patterns and where chemical groups will show up within a nuclear magnetic resonance spectrum, simply based on what else is nearby and the shielding or deshielding effects of those other groups. We now know the structure of our chemical compound.

00:10:16:52 - 00:10:38:50
Instructor: It is going to be a one, two, three carbon chain that is a CH3, CH3 on the other side, a CH in the middle with a chlorine attached at position two. The name of our compound is two chloropropane.