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# Example Analysis Using Both IR and H-1 NMR

## Transcript

Instructor: Brett McCollum

00:00:00:08 - 00:00:25:96
**Instructor:** Okay. For this video, before you watch any further, I want you to make sure that you've given it a good attempt to see whether or not you can figure out the unknown compound. If you haven't worked through it yet, make sure to pause the video here, go give it a try and then come back in about 10 minutes and see how far you've gotten. All right. We're now ready to try the problem.

00:00:25:96 - 00:00:47:40
**Instructor:** We've been given the molecular mass of our compound at 70 atomic mass units. We have our NMR spectrum shown here, and we also have an IR spectrum. Let's take a look at that. What did you see in the IR spectrum? There's something particularly important.

00:00:47:40 - 00:01:13:54
**Instructor:** We have a peak around 1,700 wave numbers. That tells us that we have a carbonial group present in our molecule. Let's make note of that that in our IR, we see a C double bond O vibration. All right. Now we're ready to build our NMR table and see what other information we can extract.

00:01:23:06 - 00:01:52:91
**Instructor:** We have our table complete. We see our chemical shifts, that signal A is at about 2 PPM, and signal B is at about 3 PPM. We haven't been given our integrations for our signals. But looking at it, I see that if we added up the heights of our peaks, we get approximately a one to two ratio for signal A to B. Then we have our multiplicity, which is a is a multiplet.

00:01:52:91 - 00:02:04:15
**Instructor:** It looks to be five peaks. A quintet. B with three peaks of height one to two to one is a triplet. That's our information. Now. Let's see if we can

00:02:04:15 - 00:02:32:34
**Instructor:** start using that to solve our problem. This one's a little interesting because we see that signal A within integration of one has how many neighbors. It's a quintet. It should have four neighbors. But do you see something with an integration of four anywhere in our spectrum?

00:02:33:06 - 00:02:59:34
**Instructor:** No. Similarly, we have signal B, an integration of two that is a triplet. That tells us that it has how many neighbors, if it's a triplet. I should have two neighboring protons. But where else would there be two protons?

00:02:59:72 - 00:03:37:95
**Instructor:** Since there's only two signals, and that is all of the protons in our molecule, we can actually see that this integration is a ratio. It is not the actual number of protons responsible for each signal. We need to double those numbers to find the number of protons in each equivalent set. That A isn't one proton, it's actually two. And B isn't two protons, it's actually four, that's how signal A has four neighbors.

00:03:37:95 - 00:04:05:05
**Instructor:** It's neighboring B, and that's how B has two neighbors, it's neighboring A. Let's start fitting this together. A appears to be a CH2 group. We know that that will have two other bonds to complete the octet of the carbon. This is equivalent group A.

00:04:05:05 - 00:04:49:63
**Instructor:** We said that it is bonded to four neighboring protons. The only other protons are these ones, of which, yes, there are four of them, but you can't put four protons on a single carbon and have it attached to the rest of the chain. This must be a CH2 and a CH2, and those CH2s have to be equivalent to each other because they show up in the same signal. We've got signal A here. We've got signal B here and here, and each of those should have one more bond to them.

00:04:50:79 - 00:05:14:16
**Instructor:** But nothing else in this compound has any more protons. What are we going to put? We know that there is a C double bond, carbonial group. That could go on one of the sides. What else is there? Let's use this information,

00:05:14:16 - 00:06:07:50
**Instructor:** our molecular mass and see if we can figure out what's going on here. If we have one, two, three carbons, three carbons each at the mass of 12 plus six hydrogens, that gives us 36 and 6,  42 atomic mass units. Now, we also have a carbonial group, that's a carbon and oxygen, 12 and 16, plus 12 more and 16 for the carbonial group, that adds up to 70 atomic mass units. There are no other atoms present in this molecule. We've filled the mass of our compound.

00:06:07:50 - 00:06:46:65
**Instructor:** We have a CH2 attached to a CH2 attached to a CH2, which is attached to a C double bond O. Well, let's build our chemical formula now. We've got C, one, two, three, four. We have six hydrogens, and we have one oxygen that added up to 70 atomic mass units. Let's determine a degree of unsaturation.

00:06:46:65 - 00:07:18:94
**Instructor:** The degree of unsaturation would be two times the number of carbons plus two minus the number of hydrogens. There are no nitrogens or halogens to worry about. We divide by 2, and we have 8 plus 2 more is 10, subtracting six is 4, divide by 2 is 2. We have a degree of unsaturation of two. One of those degrees of unsaturation is used for the carbonyl group.

00:07:19:10 - 00:07:45:40
**Instructor:** What's the other one used for? It could only represent a double bond or a ring. Ah, and that's what it is. One of our degrees of unsaturation is for this double bond. The other degree of unsaturation is because we have a ringed compound, and there's the answer.

00:07:45:40 - 00:08:12:91
**Instructor:** Our unknown compound is cyclobutanone. Hopefully, you were able to get it, but if not, assess how far you got through this problem before getting stuck and think about what are the steps that you can take next time so that you don't get stuck and you're going to get all the way to the answer of the problem. Keep trying. Good luck.