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Using IR to Predict Molecular Structure

Transcript

Instructor: Brett McCollum

00:00:00:00 - 00:00:34:26
Instructor: Infrared spectroscopy is an important tool in the tool kit for scientists to be able to identify unknown compounds. We're going to examine an IR spectrum today, and we've been given a little bit of information to get us started. We'll assume that another chemical technique has been used to determine the chemical formula of this unknown compound. Here we have our spectrum. Where do we even begin? How do you interpret a spectrum?

00:00:34:26 - 00:01:19:52
Instructor: An infrared spectroscopy spectrum, when we use the term peak, we really mean these, which you might have called valleys. But it's that our intensity of the signal is essentially measuring down along that vertical axis. We have a large peak here, a peak here, and so on. Let's see what we can gather as information out of this, relate it to our chemical formula, and see how close we can get to identifying possible options for our unknown compound. Now, keep in mind that infrared spectroscopy, its purpose within our tool kit is generally not to uniquely identify a compound.

00:01:19:52 - 00:02:15:42
Instructor: It doesn't have enough information to give us that unique identification in most cases unless you have a database to look over here within the fingerprint region to uniquely identify that compound. Rather, the main purpose of using infrared spectroscopy is instead to identify the functional groups that are present within your compound, and then you can use other pieces of information fitting the puzzle together to determine as far as you can, in terms of what your compound might be. Let's take a look. Here I see some interesting peaks, but the first one that always catches my eye is going to be right here. This peak that's close to 1,700 or 1,750.

00:02:15:42 - 00:03:13:18
Instructor: That corresponds with an important functional group in organic chemistry. If you need to, pause the video here, get out your spectroscopy data table and check what functional group should appear around 1,700 to 1,750 wave numbers. Now that you have that, what group did you find? Ideally, you're going to agree with me that this corresponds

with a carbon double bonded to an oxygen, and that is our stretching vibration for that type of bond. In particular, your data table identifies different types of carbonyl groups, whether it is a ketone, aldehyde, carboxylic acid, ester, and so on.

00:03:13:18 - 00:03:47:25
Instructor: That will slightly shift the position of the signal depending on the chemical environment. But keep in mind, other groups within the molecule can also cause electron withdrawing effects that can shift the strength of that bond and thus shift the position where it shows up in our spectrum. We want to be careful about over interpreting the parameters or the ranges given within that data table. We see that there's going to be C double bondo. There's another peak here.

00:03:47:25 - 00:04:56:24
Instructor: But before we go further, maybe we should go back to our chemical formula and pause for a moment. When we have a chemical formula given to us, there's an important technique that we can use that can also guide our decision making, and that's the determination of our degrees of unsaturation, or sometimes we call that the index of hydrogen deficiency. Our degree of unsaturation is going to be two times the number of carbon atoms plus two. We need to add in any nitrogens that are present, subtract hydrogens and halogens, and then divide by two. In our case, we have three carbons, so two times three plus two, and then we subtract our six hydrogens, and that gives us a degree of unsaturation of one.

00:04:56:49 - 00:05:32:75
Instructor: That tells us that there is either one double bond or one ring. Because we've already identified that there is a carbonial group present in our compound, we have now used up that double bond. There are no other double bonds, there are no rings in our compound. One of the carbons of the three is used for that carbonial group. One of the oxygens is used for it, but there's another oxygen present.

00:05:32:75 - 00:05:54:61
Instructor: That makes us start to think, is that other oxygen going to be in the middle of a carbon chain? Is there an ether or an ester present? Is it on the end of the carbon chain? Is it an alcohol? Or are the carbonyl group and the alcohol right beside one another, and does that form a carboxylic acid?

00:05:54:61 - 00:06:30:40
Instructor: We have some options to consider. We're looking now at this really big broad peak. In particular, look at the position where it shows up in terms of its wave numbers. This peak is a little bit higher. If we were thinking that this was a carboxylic acid, we would expect it to be between 3,400 to as low as 2,500 wave numbers, whereas this peak is above 3,500 wave numbers.

00:06:30:40 - 00:06:57:70
Instructor: This is not likely to be a carboxylic acid. Rather it matches when we say strong, we mean high intensity or a really deep peak. When we say broad, we mean the width of the peak. This is a really width peak compared to others in our spectrum. This is going to be an alcohol group.

00:06:57:70 - 00:07:31:57
Instructor: This is the stretching of that OH bond. Amines by comparison, will also show up in that same region, but they tend to have a lower intensity, and as a result, you can very quickly distinguish between what is an amine and what is an alcohol. We also see there's no nitrogen present in our chemical formula. We know that's not an option. All right. Let's start building possible structures.

00:07:31:57 - 00:07:42:57
Instructor: We have a three carbon chain. I'm going to draw that. One, two, three. When I have a three carbon chain, there is an options for splitting. This is it.

00:07:42:57 - 00:08:26:19
Instructor: Now, this carbonial group, we've decided it's not a carboxilic acid. It might be a ketone. It might be an aldehyde. We know that there's an alcohol group present, so that oxygen is used and is therefore not available for this to be right next to it as part of an ester. We don't have to worry about this carbonyl group being part of an ester or carboxilic acid.

00:08:26:19 - 00:08:41:77
Instructor: We only have two options. If we put it at the end of our chain, it'll be an aldehyde. If we put it in the middle of the chain, it's going to be a ketone. Let's try that as our first option. Here we have it in the middle of the chain.

00:08:41:77 - 00:09:09:46
Instructor: Then we need to add the alcohol group somewhere. There's only two options. I could put it there. Notice that because the alcohol group is not on the same carbon as the carbonyl group, it is not a carboxylic acid. Rather this is a compound that has two separate functional groups, the alcohol group, and the ketone group.

00:09:09:46 - 00:09:49:50
Instructor: Let's compare with our chemical formula. Always make sure you do this before you suggest this is your structure because sometimes you make a mistake and the structure you draw doesn't actually match the chemical formula that you were given at the very beginning. We expect to find three carbons, six hydrogens, and two oxygens. We have a CH3, C, O, CH2, and an OH. When I add that up together, I have three carbons, I have three, four, five, six hydrogens, and two oxygens.

00:09:49:50 - 00:10:17:65
Instructor: That matches our chemical formula. This is a possible option to match our spectrum and the information that we've been given. Now, we said other than a ketone, it could also be an aldehyde. Let's try drawing that. If I have my three carbon chain and I put

my double bond at the end on either side, and then we also have that implicit hydrogen that I've decided to show.

00:10:17:65 - 00:11:00:95
Instructor: Then we have to decide where would the alcohol go. If we put it here, that would be one option. Or we can draw the other structure where we've put the alcohol on the other available carbon. Both of these match our chemical formula, and they match the expectation that we would see in alcohol and a carbonyl group. Given that the position of our signal is around 1,720 wave numbers, that could be either a ketone or an aldehyde.

00:11:00:95 - 00:12:04:63
Instructor: We don't have enough information to distinguish which of these three is our unknown compound. If you were asked to identify a possible match for this spectrum, any of these answers would be acceptable. In this case, the correct answer that actually matches our spectrum is the ketone. But if we wanted to know that for certain, we would need to collect additional spectral information using other techniques to differentiate between these three options. Go get some more practice with IR spectroscopy, and hopefully, over time, you'll begin to see the patterns that are emerging that similar chemical bonds show up at the same places within spectra, allowing us to use IR spectroscopy to identify the functional groups that are present within organic molecules.