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Carbocation and Rearrangements

Transcript

Instructor: Sourish

00:00:00:00 - 00:00:29:72
Instructor: So today we're going to be looking at a topic that is often overlooked in organic chemistry 2, which are carbocations and carbocation rearrangements, such as using hydride and alkyl shifts. Now, since this course has a heavy focus on reactions and mechanisms, many students often overlook these concepts during their exam periods. Today we're going to be going over these concepts with three key examples, but before we do that, I want to show you a flowchart that'll help you identify three things when you're working with these examples.

00:00:31:42 - 00:00:59:62
Instructor: Now, first, it's going to help you identify what type of carbocation rearrangement you need to do, how many carbocation arrangements you need to do, and what types of carbocation rearrangements you need to do. So, whenever you are working with a carbocation in this course, I want you to pause and check if you can rearrange the carbocation to be in a more stable position before you continue with the reaction. Now, this might sound simple, but when you are stressed in your exam period, this is definitely going to be easy to forget.

00:00:59:62 - 00:01:13:72
Instructor: So do make sure you keep that in your mind. So, for this first example, we have a secondary cyclohoxyl alcohol that's reacting with HCl in room temperature. And when we refer to table 7-4, we know that this is our classic SN1 reaction.

00:01:13:72 - 00:01:27:28
Instructor: And in order to do this reaction, first, we want to protonate our alcohol group, and then we want to kick off our good leaving group to form our carbocation. And in order to do this, we can show it with our mechanism arrows. So, let's go ahead and do that first.

00:01:37:04 - 00:01:53:56

Instructor: Now that we have formed our carbocation, before we continue on with the reaction, we want to pause and check if this carbocation is at its most stable position on the molecule. So, in order to do this, an easy way is just to label all of the carbons on the molecule. So, let's go ahead and do that first.

00:01:54:72 - 00:02:22:56
Instructor: So here we can see our original carbocation position is on a secondary carbon, while the most stable position on this molecule is our tertiary carbon right here. Now, since our most stable position is not a quaternary carbon with at least one methyl group, we know that we don't need to use any alkyl shift. And next what we want to do is check how many bonds are between the original carbocation position and our more stable position, which in this case, is just one bond, as we can see right here.

00:02:22:56 - 00:02:51:44
Instructor: So, we only need to use one hydride shift. So, let's go ahead and show that by drawing our hydride in our most stable position and showing our mechanism arrows, starting from the bond of the hydride and ending on the carbon of the carbocation. Now, a common mistake many students often make is not clearly indicating the mechanism arrows starting at the bond of the hydride and ending on the carbon of the carbocation.

00:02:51:44 - 00:03:11:10
Instructor: Now, this is very important for you to do. Now, another common mistake many students make is not showing the shifted hydride once you've done your hydride shift. Now, depending on your instructor, they would most likely want you to show the shifted hydride only in the step that immediately follows your hydride shift.

00:03:11:10 - 00:03:28:78
Instructor: Let's go ahead and show that. But do double check this with your instructor on how they would like you to show your moved hydride. Now, we can continue on with our nucleophilic attack and get our SN1 products.

00:03:31:41 - 00:03:52:77
Instructor: Now, here we have our SN1 products after we have rearranged our carbocation to the most stable position. Okay, so for this second example, here we have our secondary alcohol that's reacting with HCl in room temperature. And when we refer to table 7-4, we know that this is an SN1 reaction again, like with our previous example.

00:03:52:77 - 00:04:21:63
Instructor: So likewise, what we want to do first is protonate our alcohol group to form a better leaving group, and then we can kick it off our molecule to form our carbocation. So, let's show that with our mechanism arrows. Now that we formed our carbocation, what we want to do first is label all of our carbons to check if this carbocation is at its most stable position. So, let's go ahead and do that.

00:04:24:52 - 00:04:50:78

Instructor: Now, we can see that our original carbocation is at a secondary position, while our most stable carbon is our quaternary carbons with three methyl groups. Now, according to our flow chart, since our most stable position is a quaternary carbon with at least one methyl group, this means that we will need to use an alkyl shift for our final carbocation rearrangement. Next, what we want to do is check how many bonds are between the original carbocation and our most stable position.

00:04:50:78 - 00:05:01:62
Instructor: In this case, we only have one bond. So, you only need to do one carbocation rearrangement, which is accounted for by our alkyl shift. So, what we need to do now is just simply do our alkyl shift.

00:05:01:62 - 00:05:21:68
Instructor: For alkyl shifts, what you want to do is choose one of the methyls on the quaternary carbon and denote which methyl you've chosen with a symbol. A simple dot should do. Next, what we want to do is show our mechanism arrows, and the mechanism arrows for an alkyl shift is pretty similar to a mechanism arrows for a hydride shift.

00:05:21:68 - 00:05:54:88
Instructor: So, what you want to do is start at the bond of the methyl you've chosen and end the mechanism arrow on the carbon of the carbocation. Now that we have rearranged our carbocation to be in a more stable position, we can continue with our nucleophilic attack and get our SN1 product. Likewise, we have to use our mechanism arrows to do our SN1 product.

00:05:59:01 - 00:06:13:79
Instructor: Now here is our SN1 product. Similar to a hydride shift, you don't need to show the dot that denotes the shifted methyl in the step that comes right after the alkyl shift. But do also double check this as well with your instructor.

00:06:13:79 - 00:06:39:73
Instructor: Once we have rearranged the carbocation the most stable position, now we have our SN1 product, and I just want to recap, I just want to say something again about this. Once you have done an alkyl shift, you only have to denote the symbol only in the step right after the alkyl shift. Let's say there were more steps beyond this, you don't have to show the symbol that denotes the alkyl shift, similar to how you don't have to show the hydride for a hydride shift.

00:06:39:73 - 00:07:01:65
Instructor: So, for our final example, we have a secondary alcohol that's reacting under heated and acidic conditions. And when we refer to table 7-4, we know that this is our classic E1 reaction. So in order to do our E1 reaction, we would protonate our alcohol and then kick off the good leaving group to form our carbocations, similar to the two reactions that we've previously done.

00:07:09:69 - 00:07:32:10

Instructor: Now that we formed a carbocation, what we want to do is label all of our carbons to check if our current carbocation is at its most stable position. So, like with the previous examples, let's go ahead and label all the carbons. So, we can now see that our original carbocation is at a secondary site.

00:07:32:10 - 00:07:46:92
Instructor: Well, our most stable position is a quaternary carbon with at least one methyl group. Now, here in this example, we have three methyl groups, which is good. So that means that we need to use an alkyl shift for our final carbocation arrangement.

00:07:46:92 - 00:08:18:93
Instructor: Now, what we want to do next is check how many bonds are between our original carbocation position and our more stable position. In this case, we have two bonds, so we need to do two carbocation arrangements where the first one is already counted for by our alkyl shift, and the second carbocation arrangement is done by a hydride shift. What we want to do first is show our hydride shift, like we've done in our first example by drawing our hydride in this carbon right here and showing the hydride shift with a mechanism arrow. Let's do that first.

00:08:28:29 - 00:09:07:41
Instructor: Now that we've done our hydride shift, next, we can do our alkyl shift in a similar manner to our second example where we have to denote the methyl that we have chosen on the quaternary carbon with a symbol and then we can chart our mechanism arrow from the bond of the methyl and end on the carbon of the carbocation. Let's start that. Now that we've done our alkyl shift and our carbocation is at its most stable position, we can continue on with the reaction by doing our E1 mechanism arrows, starting from the conjugate base right here and ending on the Beta hydrogens of this carbocation.

00:09:07:41 - 00:09:41:12
Instructor: Once we do that, we can find our E1 products, and then thereafter, we can determine our major and minor products if needed. Okay. After we've done our carbocation rearrangement and our E1 reaction, now we have our correct major and minor products.

00:09:41:12 - 00:10:06:46
Instructor: Now, like we've learned last semester in Organic Chem one, we know that this one is our major product because it's more substituted. This double bond is connected to four bonds right here, carbons right here, this is our minor product because it is less substituted, and this double bond is connected to only two carbons right here. Now as we wrap up the video today, I want you to keep three things in mind when you're working with carbocations in this course.

00:10:06:46 - 00:10:22:58
Instructor: First, I want you to keep in mind, can this carbocation rearrange to be in a more stable site? Is that more stable site a quaternary position with at least one methyl groups? I

want you to check how many bonds are between the original carbocation site and the more stable site.

00:10:22:58 - 00:10:38:63
Instructor: Now, like I said, in the introduction, this course can seem very intimidating at the start since you have to memorize a lot of reagents and a lot of different reactions. However, it will become second nature. It will become second nature to you if you keep on practicing and keep on trying.

00:10:38:63 - 00:10:50:25
Instructor: I also advise you to go check in with your instructor if you do need help. I hope this video made this concept a little bit easier for you. Good luck with your exams, and thank you.