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Benzene Electrophilic Aromatic Substitution

Transcript

Instructor: Emily

00:00:00:00 - 00:00:22:16
Instructor: Everyone, today, we're going to be talking about benzene EAS, and it's where an aromatic ring acts as a nucleophile and replaces proton with an electrophile to restore aromaticity. So a carbon hydrogen bond is broken.

00:00:26:60 - 00:00:48:32
Instructor: And a carbon bond is formed with an electrophile. So the first step involves an electrophilic attack.

00:00:48:32 - 00:01:01:94
Instructor: So the Pi electrons from the double bond are donated to the electrophile Í

00:01:10:97 - 00:01:24:69
Instructor: The second step involves loss of a proton. So the electrons form a double bond, restoring aromaticity.

00:01:24:89 - 00:01:43:38
Instructor: And just as a reminder, This is a hinder. To be aromatic, to be planar, conjugated, cyclic, and it has to follow Huckel's rule, which this molecule does.

00:01:43:78 - 00:01:48:80
Instructor: So there are five types of EAS. The first is Halogenation.

00:01:48:80 - 00:02:02:58
Instructor: Also, you might see it as bromination and chlorination, Nitration, Sulfonation, Alkylation, and Acylation. So first, we'll go over bromination.

00:02:15:79 - 00:02:30:11
Instructor: So the first one is bromination, and as you can see, we have bromine. And so the electrophile here is BR plus.

00:02:33:83 - 00:02:42:99

Instructor: The second one is chlorination, and as you can see, it's very similar to bromination. So if you can remember one, you can remember the other.

00:02:43:83 - 00:02:59:43
Instructor: So here, the electrophile would be chlorine plus. I think that's a big tip in organic chemistry is to really notice patterns because then you don't have to remember as much and it feels less overwhelming.

00:02:59:43 - 00:03:08:41
Instructor: So next up, we have nitration here and sulfonation on the bottom. And I put these two together so you can notice some patterns.

00:03:08:41 - 00:03:21:32
Instructor: Both of them use sulfuric acid as the catalyst. Yeah.

00:03:21:32 - 00:03:43:52
Instructor: So in nitration, the electrophile is NO2+, and then in sulfonation, the electrophile is SO3+. Sulfuric acid protonates nitric acid to activate it, and then it loses water to form NO2, which is why we have NO2 plus as our electrophile.

00:03:43:52 - 00:04:02:10
Instructor: And then down here for sulfonation, you'll notice we have an extra hydrogen on the end, and this is because SO3+ isn't stable on its own, so it gets protonated by the sulfuric acid. Next up, we have alkylation and acylation.

00:04:02:16 - 00:04:10:70
Instructor: And I pair these together because there's more patterns. So as you can see, they have the same catalysts.

00:04:10:70 - 00:04:31:96
Instructor: And so for alkylation, the electrophile for alkylation, the electrophile is R+. Then in acylation, the electrophile is ROC+ because the carbon carries the positive charge.

00:04:31:96 - 00:04:41:16
Instructor: So next step, we have activating and deactivating groups. So I've made this lovely little table for you to help you when you're studying.

00:04:41:16 - 00:04:54:02
Instructor: So we'll start off with electron donating groups EDG. They are activating because they're electron donating, so they're putting electron density into the ring.

00:04:54:02 - 00:05:07:61
Instructor: And because they're activating, that means it speeds up the reaction. The activators are also ortho-para directors, and here we have some examples.

00:05:07:61 - 00:05:31:53

Instructor: Next up, we have electron withdrawing groups, EWG, so these are deactivating groups because they're taking electron density away from the ring, therefore slowing the reaction down. Electron withdrawing groups and deactivators are also metadirectors.

00:05:31:53 - 00:05:40:65
Instructor: And here we have some examples. But it wouldn't be organic chemistry without an exception.

00:05:40:65 - 00:05:55:43
Instructor: So for halogens, even though they're electron withdrawing groups, they are still deactivating, but they are ortho-para directors instead of meta directors. And they slow down the reaction.

00:06:00:31 - 00:06:22:01
Instructor: And just as a reminder for Ortho, Meta, and Para directors, if we have R group here, the Ortho is directly beside it, and then Meta is next, and Para is last. And I noticed when I was making this, it spells out m. So if you can't remember,

00:06:22:01 - 00:06:33:47
Instructor: oh, is this one Meta, Para Ortho, spell. So now we'll move on to some practice problems.

00:06:33:47 - 00:06:47:97
Instructor: So for the first one here, we need to predict the reagents. So we have SO3H. So we know the for this one,

00:06:47:97 - 00:07:00:97
Instructor: we know the electrophile is SO3+ because it's sulfonation. And then we have to remember the sulfuric acid because that's what protonates the SO3+.

00:07:00:97 - 00:07:12:31
Instructor: The next one, we have a nitration since we have NO2. So the electrophile is NO2+.

00:07:12:31 - 00:07:26:23
Instructor: But remember, we lose a water, so we need to have we need to have nitric acid, so HNO3. And remember, sulfonation and nitration.

00:07:26:23 - 00:07:41:10
Instructor: They both have sulfuric acid as a catalyst. So when you see questions like this, first think, which of the five EAS is this?

00:07:41:10 - 00:07:49:08
Instructor: And because we have SO3H, we know that it's a sulfonation. So that's why we put SO three.

00:07:49:08 - 00:08:00:11

Instructor: And then, again, we need the sulfuric acid in order to protonate the SO three. And same goes for this one.

00:08:00:11 - 00:08:22:15
Instructor: We look at all the different options, and we know it's nitration because we have NO2. And as a check, you can always go back to your two step mechanism, as we see, we have SO3+ as our electrophile, and we're forming a carbon bond to the electrophile, which we have here.

00:08:22:15 - 00:08:30:53
Instructor: So next up, we have a predict the product question. And the first step is to decide what kind of EAS we have.

00:08:30:53 - 00:08:42:73
Instructor: And because we have BR2, we know it's a bromination, which is a type of halogenation. But we need to decide where the bromine goes.

00:08:42:73 - 00:08:50:35
Instructor: And we have three possible options here. We'll start off here with this R group.

00:08:50:35 - 00:09:03:33
Instructor: And since all of the alkanes are metadirectors, this is our R group, so like right here. And then we have an ortho position and a meta position.

00:09:03:33 - 00:09:10:05
Instructor: The bromine most likely won't be here since there's already a substituent there. So let's go the other way around the ring.

00:09:10:05 - 00:09:18:17
Instructor: So we have the R group and then ortho and meta. So that's a possibility. But we're not done.

00:09:19:58 - 00:09:25:88
Instructor: Now, let's start with this R group. So we have ortho and meta.

00:09:25:88 - 00:09:36:06
Instructor: Now there are two, but we need to go the other way too. Ortho, meta, and again, there's already a substituent there, so it most likely won't be there.

00:09:36:42 - 00:09:46:52
Instructor: And now for the last R group, go ortho, meta. So it could be there, ortho, meta.

00:09:46:52 - 00:10:04:16
Instructor: So now, looking at where all the possible options are for the bromine, this position has two dots, so we will put the bromine there. So this would be your final answer.

00:10:04:16 - 00:10:13:14

Instructor: For the last practice question, it's another predict the product. And first off, we have to decide, what kind of EAS is this?

00:10:13:14 - 00:10:30:24
Instructor: So we go through, and you see here that it's COCL so we'll have an insulation. And this is the alkane is a meta director again.

00:10:30:24 - 00:10:47:98
Instructor: So we have this is the R group, ortho, meta and then ortho, meta. So you could have two answers, but they're technically the same because the molecule is symmetrical, so you just have to list one.

00:10:47:98 - 00:11:00:98
Instructor: Then this would be your final answer. So just remember when you are trying to predict the products for these types of questions, first, decide what type of EAS this is.

00:11:00:98 - 00:11:23:90
Instructor: And next, use your table to see if it is a deactivating or an activating group, so you know where to put the substituent. Additionally, you can also look at the mechanism so you have a better idea of what is going on in order to predict the final product.