



S_N1 and S_N2 Competition

Transcript

Instructor: Brett McCollum

00:00:00:00 - 00:00:23:02

Instructor: In this video, we're going to now look at nucleophilic substitution, and we don't know if it is going to be an S_N1 or an S_N2 pathway. We need to decide that. We look at our initial compound, and we also have our solvent here. Looking at this, where's our leaving group? Right here, it's the chlorine.

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Instructor: The chloride is going to leave taking that electron pair, leaving behind a carbon that will be positively charged. We check what type of carbocation are we going to form. It's going to be tertiary. That suggests that this might be an S_N1 pathway because that's a stable carbocation. The leaving group, is a good leaving group and leaves behind a stable intermediate.

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Instructor: Let's also check what will be our nucleophile. What else is in the system? A solvent. In this case, the solvent is acting as both solvent and nucleophile. We call this solvolysis.

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Instructor: This is not negatively charged. It's not going to be a strong nucleophile. It's not going to be good at pushing out the leaving group, that would be S_N2. Rather, it's going to wait till the leaving group has left, and then attack our carbocation. That's why this is preferred for a S_N1 pathway.

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Instructor: Additionally, our solvent is polar protic. That's good at stabilizing the intermediate carbocation. All of these factors together, tell me this is going to be a S_N1 pathway. Let's start drawing. We have the electron pair between the carbon and the chlorine, and that bond is going to break forming our initial carbocation in step one of this reaction.

00:02:12:56 - 00:02:54:80

Instructor: Now, notice that we went from a chiral center, this would have been the S enantiomer to now having a trigonal planar geometry for our carbocation and our nucleophile can attack from either above or below. As a result, that is going to change what we have for our stereochemistry. We're going to go from a specific stereochemical center here to both options forming, a racemic mixture. Let's draw that step. An electron pair now attacks our carbocation.

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Instructor: We could draw it here on this side or on the other side, and we form our next intermediate species. Now, if it formed from attack from above or below, you just need to draw the methyl and your oxygen with one pointing up, one pointing down. But in this case, because I know a racemic mixture is forming, I didn't bother indicating that stereochemistry because both options occurred. We have a species now that has a positively charged oxygen, you may recall, we call these an oxonium ion. This is an unstable reaction intermediate.

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Instructor: We need to stabilize it. How do we do that? Generally, we need to get rid of that proton. We're going to undergo an acid base reaction, transferring that proton to another species. What is in our system that could serve as an electron donor and receive that proton?

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Instructor: Remember the chlorine, I came off as a chloride ion, and it's still there in our system, and we can use it to abstract this proton, moving the electron pair up onto the oxygen, forming our final product. And we have our byproduct of hydrogen chloride. What did we do in this reaction? We transformed a halogenated hydrocarbon into an ether via an SN1 pathway.