Nucleophilic Aromatic Substitution (SNAR)

Transcript

00:00:00:28 - 00:00:10:54
Dr.Jessie Key: Hello again, Dr. Jessie Key here. In this video, you'll be exploring the nucleophilic aromatic substitution or SNAR mechanism.

00:00:10:54 - 00:00:49:50
Dr.Jessie Key: SNAR's proceed through a two-step reaction mechanism: nucleophilic attack, followed by loss of leaving group. Let's push some arrows and see how this mechanism occurs: Starting with a substrate of 1-bromo-4-nitrobenzene, notice we have a good leaving group, bromine that is para to the strong electron withdrawing nitro group. Here the nucleophile is hydroxide, which performs a nucleophilic attack on the ring carbon bearing the leaving group.

00:00:51:10 - 00:01:20:45
Dr.Jessie Key: The pi bond between carbon 1 and 2 moves to become a lone pair on carbon 2, giving it a formal negative charge. This resonance stabilized intermediate is known as a Meisenheimer complex. Several resonance contributors can be drawn for this Meisenheimer complex, including one where we move the electrons down onto the electron-withdrawing nitro group.

00:01:20:45 - 00:01:54:47
Dr.Jessie Key: First, we can move the lone pair from carbon 2 to form a new pi bond between carbon 2 and 3. The existing pi bond between carbon 3 and 4 moves on to carbon 4, giving the next resonance contributor. We can then perform a similar pattern to get to our next resonance contributor by moving the lone pair to form a new pi bond between carbon 4 and 5, moving the existing pi bond between carbons 5 and 6 onto carbon 6.

00:02:08:50 - 00:02:47:19
Dr.Jessie Key: The final resonance contributor can be obtained by bringing that lone pair of electrons down to re-form the pi bond between carbons 5 and 6 and move the pi bond between carbon 4 and 5 to form a new carbon-nitrogen double bond. This moves the nitrogen-oxygen pi bond down onto the oxygen to become a new lone pair and a formal negative charge. The second step of SNAR mechanism is loss of the leaving group, and we can show that from any of the resonance contributors.

00:02:47:19 - 00:03:22:31

Dr.Jessie Key: But in this case, let's use the last one we drew that has the extra electron density down on the nitro group. Starting at the oxygen lone pair we just created, we can re-form the nitrogen-oxygen Pi bond, move the carbon nitrogen double bond to form a new Pi bond between carbons 3 and 4, and then move the existing pi bond between carbons 3 and 2 up to form a new pi bond between carbons 1 and 2. This causes the carbon-bromine sigma bond to break and form a new lone pair on the bromine atom to result in loss of the leaving group bromide anion.