Birch Reduction Mechanism and Predicting Products

Transcript

00:00:00:00 - 00:00:09:66
Dr.Jessie Key: Hello again, Dr. Jessie Key here. In this video, you'll be exploring the Birch Reduction Mechanism, and its use to predict the products of a birch reduction.

00:00:09:66 - 00:00:33:84
Dr.Jessie Key: The Birch reduction proceeds through a dissolving metal type mechanism, similar to that used in the reduction of alkynes. It features four steps: In the first step, a nucleophilic attack is performed by a lone electron from sodium. A fish hook arrow is used starting at the electron on the sodium, having it go to form a new lone pair of electrons on one of the carbons of benzene.

00:00:34:37 - 00:01:05:37
Dr.Jessie Key: An existing pi bond within benzene breaks with one electron supplying the other electron for the new lone pair and the other electron coming down to form a new pi bond. Another pi bond in benzene breaks, and one electron goes to complete the new pi bond with the other going to form a radical on the carbon para to the one where the lone pair formed. This gives a radical anion intermediate.

00:01:10:41 - 00:01:39:17
Dr.Jessie Key: In the second step, a proton transfer occurs with the newly formed lone pair of the radical anion abstracting a proton from the solvent methanol. This results in a radical intermediate. The radical intermediate undergoes another nucleophilic attack from another sodium molecule to generate an anionic intermediate.

00:01:44:09 - 00:02:29:66
Dr.Jessie Key: The mechanism is finished by a second proton transfer with the methanol solvent to give the cyclohexa 1cyclohexa-1,4-diene product Notice that although the mechanism is technically four distinct steps, it is essentially the same two steps repeated twice. Nucleophilic attack by the sodium radical, followed by a proton abstraction from the methanol solvent. Another thing to note about the birch reduction is that the final products

end up with two sp3 hybridized carbons opposite to each other on the newly formed cyclohexadiene ring.

00:02:31:08 - 00:03:01:32
Dr.Jessie Key: The regioselectivity of this reduction can be affected by the presence of substituents on the starting aromatic ring. When an alkyl electron donating group like a methyl is present, the carbon bearing the methyl is not reduced. While the presence of an electron withdrawing substituent like a ketone provides the opposite regiochemical outcome.

00:03:02:99 - 00:03:29:49
Dr.Jessie Key: This regioselectivity arises from the anionic nature of the intermediates in the mechanism. The presence of electron donating substituents at the carbon bearing the anion will further destabilize the radical anion and anion intermediates. However, the presence of an electron withdrawing group will help to stabilize the anionic intermediates.

00:03:29:49 - 00:03:44:63
Dr.Jessie Key: Let's take a look at an example problem, predict the major product for the following Birch reduction, and explain your choice. Take a moment, pause the video and try this on your own first. We'll go through this together after you're ready.

00:03:49:45 - 00:04:18:71
Dr.Jessie Key: The starting material has an ethyl substituent and a methyl ester. The ethyl group will be electron donating and therefore we should not expect reduction at that carbon. The ester group has a carbonyl, which is electron withdrawing, it should stabilize the anions formed during reduction at that position.

00:04:18:71 - 00:04:29:97
Dr.Jessie Key: The expected major product would therefore be the cyclohexadiene, with the carbonyl adjacent ring carbon and the ring carbon opposite sp3 hybridized.