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Predicting Diels-Alder Reaction Products

Transcript

00:00:00:00 - 00:00:09:58
Dr.Jessie Key: Hello, again, Dr. Jessie Key, here. In this video, we will be exploring how to determine the expected products for Diels-Alder reactions by working through a few examples.

00:00:09:58 - 00:00:42:34
Dr.Jessie Key: In our first example, we're given the following reactants: buta-1,3-diene and dimethyl but-2-ynedioate. The first thing we should do is identify the diene and dienophile. In this case, we have buta-1,3-diene acting as the diene, and the alkyne dimethyl but-2-ynedioate can serve as our dienophile because it has a pi bond and ester electronic drawing groups.

00:00:42:50 - 00:01:17:33
Dr.Jessie Key: I find it really helps for pericyclic reactions like cycloadditions, to number my carbons and then take the time to draw the curved arrow notation mechanism to help me keep track of the bonds which are being formed, broken, or moved. I've numbered the carbons of the diene from 1 to 4, and the carbons involved in the mechanism from the alkyne as 1’ and 2’. The reaction goes through the cyclic transition state, and we can show the new bonds forming with dash lines.

00:01:18:41 - 00:01:45:38
Dr.Jessie Key: My arrows are starting at the electron source of the pi bond of the alkyne to form a new sigma bond to carbon 1 of the diene. The pi bond between carbon 1 and 2 of the diene moves to form a new pi bond between carbons 2 and 3. The pi bond between carbons 3 and 4 of the diene goes to form a new sigma bond between carbon 4 and carbon 2' prime of the alkyne.

00:01:45:38 - 00:02:20:80
Dr.Jessie Key: This gives the following Diels-Alder product, which is a cyclohexadiene diester. The second example again has buta-1,3-diene acting as the diene. It's just drawn in its s-trans conformation.

00:02:20:80 - 00:02:51:54

Dr.Jessie Key: The dienophile is (2Z)-but-2-enedial, an alkene with two aldehydes arranged cis relative to the pi bond. I'll first redraw these structures to help facilitate the mechanism proceeding through the cyclic transition state. Now buta-1,3-diene is shown after adopting its s-cis conformation with carbons numbered as before, and the dienophile has been rotated.

00:02:51:54 - 00:03:17:08
Dr.Jessie Key: I start my arrow at the electron source of the pi bond of the dienophile to form a new sigma bond to carbon 1 of the diene. The pi bond between carbon 1 and 2 of the diene moves to form a new pi bond between carbons two and three. The pi bond between carbons 3 and 4 of the diene goes to form a new sigma bond between carbon 4 and carbon 2' prime of the dienophile.

00:03:29:94 - 00:04:07:58
Dr.Jessie Key: This gives the cyclohexene product shown, which has the two aldehydes relatively cis since the dienophile was a cis-disubstituted alkene. The final example on this video has cyclopentadiene acting as the diene and (2Z)-but-2-endioic acid as the dienophile. Once again, I start by numbering the carbons involved in the mechanism transition state.

00:04:09:10 - 00:04:36:06
Dr.Jessie Key: I start my arrow at the electron source of the pi bond of the dienophile to form a new sigma bond to carbon one of the diene. The pi bond between carbon one and two of the diene moves to form a new pin between carbons 2 and 3. The pi bond between carbons 3 and 4 of the diene goes to form a new sigma bond between carbon 4 and carbon 2' prime of the dienophile.

00:04:43:12 - 00:05:12:60
Dr.Jessie Key: Notice that the product formed is a bicyclic system. This means the major product will be the Endo product, having the carboxylic acid electron withdrawing substituents placed syn to the larger ring of the bicyclic structure. Remember, endo is preferred due to the stabilizing interaction between newly developing bonds and the electron withdrawing groups.