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Predicting Diels-Alder Reaction Products

Transcript

Instructor: Jessie Key

00:00:00:00 - 00:00:28:10
Instructor: Hello, again, Doctor Jesse Key, here, in this video, we'll be exploring how to determine the expected products for Diels-Alder reactions by working through a few examples. In our first example, we're given the following reactants, Butta one, three diene and dimethyl but-2-ine-dioate. The first thing we should do is identify the diene and dienophile.

00:00:28:10 - 00:01:08:21
Instructor: In this case, we have Buta 1,3 diene acting as the diene, and the alkyne dimethyl but-2-ine-dioate can serve as our dienophile because it has a Pi bond and Ester electronic drawing groups. I find it really helps for paracyclic 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 1-4, and the carbons involved in the mechanism from the alkyne as one prime and two prime.

00:01:09:81 - 00:01:36:34
Instructor: The reaction goes through the cyclic transition state, and we can show the new bonds forming with dash lines. My arrows are starting at the electron source of the Pi bond of the alkyne to form a new Sigma bond to carbon one of the diene. The pi bone between carbon one and two of the diene moves to form a new pi bond between carbons two and three.

00:01:36:82 - 00:02:16:80
Instructor: The pi bond between carbons three and four of the diene goes to form a new Sigma bond between carbon four and carbon two prime of the alkyne. 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.

00:02:16:80 - 00:02:37:24
Instructor: It's just drawn in its S trans conformation. The dienophile is two z but-2-ene dial 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.

00:02:42:44 - 00:03:07:12
Instructor: Now beta 1,3 diene is shown after adopting its cis conformation with carbons numbered as before, and the dienophile has been rotated. 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 die moves to form a new pi bon between carbons two and three.

00:03:07:92 - 00:03:59:74
Instructor: The pi bond between carbons three and four of the diene goes to form a new sigma bond between carbon four and carbon two prime of the dienophile. 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 two z but-2 and dioic acid as the dienophile.

00:04:01:34 - 00:04:25:82
Instructor: Once again, I start by numbering the carbons involved in the mechanism transition state. 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 bon between carbon one and two of the diene moves to form a new pin between carbons two and three.

00:04:26:74 - 00:04:51:82
Instructor: The pi bond between carbons three and four of the diene goes to form a new sigma bond between carbon four and carbon two prime of the dienophile. Notice that the product formed is a bicyclic system. This means the major product will be the endo product.

00:04:51:82 - 00:05:12:60
Instructor: Having the carboxylic acid electron withdrawing substituents placed sin 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.