



Alpha Fragmentation Mechanism

Transcript

00:00:00:00 - 00:00:14:28

Dr. Jessie Key: Again, Dr. Jessie Key here. In this video, we are going to talk through the Alpha cleavage fragmentation mechanism for mass spectrometry and see it applied to predict the fragmentation products for an example, alcohol.

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Dr. Jessie Key: Let's first go through the mechanism with the generic alcohol, notice we have two R groups attached, R1 and R2, making it generic. First, we need to identify the Alpha and Beta positions available. In the case of this generic example, we're just going to do that for the carbons explicitly shown.

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Dr. Jessie Key: Next, we use single barbed "fish-hook" arrows to show the flow of single electrons. Starting at the radical electron on the oxygen, we can bring an arrow down to form a new Pi bond between the oxygen and the alpha carbon, the carbon-carbon bond between the Alpha and the Beta position undergoes homolytic cleavage with one electron going to help form the new pi bond and the second electron going to the Beta position as a radical. This gives us an M-beta product ion fragment, which is resonance stabilized and a radical fragment.

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Dr. Jessie Key: Let's now take a look at the Alpha cleavage fragmentation, which would occur for this example, octan-3-ol. The Alpha position is located here at the carbon attached to the alcohol, and there are two Beta positions adjacent. If cleavage occurs between carbons 3 and 4, we can draw the mechanism, starting from the radical cation's radical electron coming down to form the new Pi bond and cleave the sigma bonds between the alpha and beta positions, carbons 3 and 4.

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Dr. Jessie Key: This would give the resulting product ion and radical fragments. Remember, the product ion will be the only one to show in the mass spectrum. If cleavage occurs between carbons 2 and 3, we can draw the mechanism starting from the radical cation's

radical electron coming down to form the new pi bond and cleave the sigma bonds between the alpha and beta positions, carbons 2 and 3.

00:02:47:92 - 00:03:00:64

Dr. Jessie Key: This would give the resulting product ion and radical fragment. Remember, the product ion will be the only one to show in the mass spectrum.