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Organic Chemistry: Synthesis of Oxacyclopentane from Cyclohexene

To understand the process of transforming cyclohexene into oxacyclopentane, the chemical reactions will be broken down into their respective steps, along with the required reagents and explanations for each part.

Step 1: Epoxidation of Cyclohexene

Given Data and Introduction:

Cyclohexene is an alkene with the chemical formula C_6H_{10} . The target product is oxacyclopentane, commonly known as tetrahydrofuran (THF), which is a 5-membered cyclic ether with the chemical formula C_4H_{80} .

Step:

Start by converting cyclohexene into an epoxide.

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Cyclohexene + Peroxyacid (e.g., m-CPBA) \rightarrow Cyclohexene epoxide
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Explanation:

The epoxidation step introduces an oxygen atom across the double bond of cyclohexene, forming a three-membered ring structure known as an epoxide. This step is a typical reaction of alkenes with peroxyacids.

Supporting statement:

Epoxidation helps in the preparation of an intermediate that can undergo further reactions to construct the desired 5-membered ether ring.

Step 2: Ring-Opening of Epoxide

Given Data and Introduction:

The next step involves the ring-opening of the epoxide to generate a more reactive intermediate.

Step

Convert the cyclohexene epoxide to a diol using acidic hydrolysis.

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Cyclohexene epoxide + H_2O, H^* \rightarrow 1,2-Cyclohexanediol
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Explanation:

Acidic hydrolysis of the epoxide ring leads to the formation of a diol, which is crucial for creating the reactive centres required for subsequent transformation.

Supporting statement:

Hydrolysis of the epoxide effectively prepares the molecule for further cyclization by generating two hydroxyl groups.

Step 3: Pinacol Rearrangement

Given Data and Introduction:

To create a 5-membered ring, the 1,2-cyclohexanediol must undergo a rearrangement known as the pinacol rearrangement.

Step:

Perform the pinacol rearrangement under acidic conditions.

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1,2-Cyclohexanediol + Acid (e.g., H^*) \rightarrow Tetrahydrofuran + water
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Explanation:

Under acidic conditions, the 1,2-cyclohexanediol undergoes a molecular rearrangement (pinacol rearrangement) resulting in the formation of a 5-membered cyclic ether and water.

Supporting statement:

The rearrangement step closes the ring to form the desired oxacyclopentane structure.

Final Solution:

Cyclohexene undergoes epoxidation using m-CPBA to form cyclohexene epoxide. The epoxide then undergoes hydrolysis to form 1,2-cyclohexanediol. Finally, through a pinacol rearrangement under acidic conditions, tetrahydrofuran (oxacyclopentane) is formed.

Reagents Required:

- 1. m-CPBA for epoxidation
- 2. Water and an acid (e.g., H₂SO₄) for hydrolysis and rearrangement.

Using a sequence of epoxidation, hydrolysis, and pinacol rearrangement, cyclohexene can be transformed into oxacyclopentane (THF) efficiently, showcasing a clear and logical approach in organic synthesis.