Experiment 15

Diels-Alder Reaction: A Reaction with High Atom Economy

Study Questions

1) Given the following reaction sequence and information, draw an energy diagram (Energy vs Reaction Coordinate) illustrating the major energetic features of the following reaction.

\[ \text{C} \quad \text{Thermodynamic Product} \quad \text{A} \quad \text{Starting Material} \quad \text{B} \quad \text{Kinetic Product} \]

Answer:

2) Provide the products for the following Diels-Alder reactions. Be sure to indicate the stereochemistry of the products where applicable.

   a. \( \text{CH}_2=CH\text{CO}_2\text{CH}_3 + \text{CH}_2=\text{CH}\text{CO}_2\text{CH}_3 \rightarrow \)
   b. \( \text{CH}_2=\text{C}(-\text{CN})_2 + \text{CH}_2=\text{C}(-\text{CN})_2 \rightarrow \)
   c. \( \text{CH}_2=\text{CH} + \text{CH}_2=\text{CH}-\text{CO}_2\text{H} \rightarrow \)
   d. \( \text{CH}_2=\text{CH} + \text{CH}_2=\text{CH}-\text{CO}_2\text{H} \rightarrow \)
   e. \( \text{CH}_2=\text{CH} + 2 \text{CH}_{2}=\text{CH} \rightarrow \)

Answer:
Experiment 15: Diels-Alder Reaction

3) The reaction shown below is an example of the Wittig reaction, which you will learn about in Chapter 19 of Loudon. What is the atom economy for this particular reaction?

\[
\text{Camphor} \quad \text{MW} = 152.24 \\
\text{Methyltriphenylphosphonium bromide} \quad \text{MW} = 357.23 \\
\text{Potassium \textit{tert}-butoxide} \quad \text{MW} = 112.21
\]

\[
\begin{array}{c}
\text{MW} = 150.26 \\
\text{MW} = 278.29 \\
\text{MW} = 74.12 \\
\text{MW} = 119.00
\end{array}
\]

(Desired product)

If a chemist performs this reaction using 0.152 g of camphor, 0.536 g of methyltriphenylphosphonium bromide, and 0.168 g of potassium \textit{tert}-butoxide, and isolates 0.138 g of product, what is the percent yield? \textbf{Answer:} The atom economy is 24.17%, and the yield is 92.0%.

4) Describe each of the following pairs of groups as homotopic, enantiotopic, diastereotopic, or chemically inequivalent.
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