Module 9: Elimination Reactions

Elimination is the reverse process to the addition reactions we saw in Week 4: it converts a haloalkane or alcohol into an alkene.

1. Complete the mechanism for the elimination of water to form propene.

   \[
   \begin{array}{c}
   \text{H}^+ \\
   \text{H} \\
   \text{OH} \\
   \rightarrow \\
   \text{H} \\
   \text{O} \\
   \text{OH} \\
   \rightarrow \\
   -\text{H}_2\text{O} \\
   \rightarrow \\
   -\text{H}^+ \\
   \rightarrow \\
   \end{array}
   \]

2. This type of elimination reaction is referred to as an E1 reaction. By comparing with the \( \text{S}_1\) and \( \text{S}_2\) reactions you have already seen, explain this nomenclature. Which step is the slowest (i.e., the rate determining step)?

3. The first step involves protonation of the alcohol. Why is this step necessary?

4. Given that more substituted alkenes are more stable (more substituents means more hyperconjugation), what would you expect to be the major product of the reaction below?

   \[
   \text{OH} \\
   \rightarrow \\
   \text{conc.} \quad \text{H}_2\text{SO}_4 \\
   \quad \text{heat} \\
   \rightarrow \\
   \end{array}
   \]

   This is an example of Zaitzev's Rule: the major product of an elimination reaction will be the more substituted alkene (when an E1 mechanism operates).

Extension: How might you achieve the transformation below? (More than one step required.)
The base catalysed elimination of HBr from a bromoalkane is an example of a different type of elimination reaction.

5. Add curly arrows to complete a mechanism for this elimination.

\[
\begin{array}{c}
\text{H} \\
\text{Br} \\
\text{H}_2\text{O} \\
\text{Br} \\
\end{array}
\quad \xrightarrow{\text{OH}} \\
\begin{array}{c}
\text{H} \\
\text{Br} \\
\text{H}_2\text{O} \\
\text{Br} \\
\end{array}
\]

6. How would you classify this reaction (in letters and numbers, like S_N1, S_N2, E1 etc)?

Because this is a concerted process (bonds made and broken at the same time), *steric effects* (the size and bulkiness of the reagents) are more important than in E1 reactions. (Compare to S_N2 reactions, which are faster for less bulky alkyl halides.)

7. Which of the hydrogens H_a or H_b is more hindered? Which one is more accessible to a bulky base like potassium tert-butoxide (KOTBu)? Predict the outcome of the following reaction.

\[
\begin{array}{c}
\text{H}_a \\
\text{Br} \\
\text{H}_b \\
\end{array}
\quad \xrightarrow{\text{KO}^\text{Bu}} \\
\begin{array}{c}
\text{H}_a \\
\text{Br} \\
\text{H}_b \\
\end{array}
\]

Does your prediction follow Zaitzev's Rule? Are you comfortable with this? Why does Zaitzev's Rule not apply in this case?

8. Predict the outcome of the previous reaction if you were to use KOH as the base.

**Extension:** Suggest a way to achieve this transformation (again more than one step is required):

\[
\begin{array}{c}
\text{H}_a \\
\text{Br} \\
\text{H}_b \\
\end{array}
\quad \xrightarrow{\text{KOH}} \\
\begin{array}{c}
\text{H}_a \\
\text{Br} \\
\text{H}_b \\
\end{array}
\]