Addition of Br₂ to trans-Cinnamic Acid: Mechanistic Investigation

Possible mechanisms for addition:

SYN

ANTI

SYN and ANTI
Addition of Br₂ to *trans*-Cinnamic Acid: Mechanistic Investigation

**SYN ADDITION**

\[
\begin{align*}
&\text{Br} & \text{Br} \\
&\text{Ph} & \text{H} & \text{CO}_2\text{H} \\
\end{align*}
\]

\[
\begin{align*}
\rightarrow &\quad \text{transition state} \\
&\quad \text{M.P. 93.5 - 95°C} \\
\end{align*}
\]

\[
\begin{align*}
&\text{Br} & \text{Br} \\
&\text{Ph} & \text{H} & \text{CO}_2\text{H} \\
\end{align*}
\]

\[
\begin{align*}
(2S,3S) + (2R,3R) \\
\text{M.P. 93.5 - 95°C}
\end{align*}
\]
Addition of Br₂ to *trans*-Cinnamic Acid: Mechanistic Investigation

**ANTI ADDITION**

(from addition of Br to top face)

(2S,3R) + (2R,3S)  
M.P. 202 - 204°C

(from addition of Br to bottom face)
Addition of Br₂ to trans-Cinnamic Acid: Mechanistic Investigation

SYN and ANTI ADDITION
### Connecting the Physical Data with the Mechanism

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Stereoisomers formed</th>
<th>Melting point</th>
</tr>
</thead>
<tbody>
<tr>
<td>syn</td>
<td>((2S,3S)/(2R,3R))</td>
<td>93.5-95°C</td>
</tr>
<tr>
<td>anti</td>
<td>((2S,3R)/(2R,3S))</td>
<td>202-204°C</td>
</tr>
<tr>
<td>syn + anti</td>
<td>((2S,3S)/(2R,3R)) &amp; ((2S,3R)/(2R,3S))</td>
<td>characteristic of a mixed sample</td>
</tr>
</tbody>
</table>

### Determining the Percent Yield

\[
\text{Ph} \quad \begin{array}{c} \equiv \ \equiv \ \equiv \end{array} \quad \text{H} \quad \text{H} \quad \text{CO}_2\text{H} \quad + \quad \text{Br}_2 \quad \xrightarrow{\text{CH}_2\text{Cl}_2} \quad \begin{array}{c} \text{Ph} \quad \end{array} \quad \begin{array}{c} \equiv \ \equiv \ \equiv \end{array} \quad \text{Br} \quad \text{Br} \quad \text{CO}_2\text{H} \quad \\
\text{MW 148.16} \quad \text{C}_9\text{H}_8\text{O}_2 \quad \text{MW 159.81} \quad \text{MW 307.97} \quad \text{C}_9\text{H}_8\text{Br}_2\text{O}_2 \quad \\
\]

Which reagent is the limiting reagent?
Tips and Reminders

1. Avoid resting the reaction flask directly on the surface of the heating mantle

2. Reflux the solution until all the *trans*-cinnamic dissolves – then start adding bromine

3. The product should begin to precipitate relatively quickly

4. Use only the minimum amount of cold CH₂Cl₂ to wash the crude product

5. The reaction filtrate constitutes halogenated waste

6. In the lab report, the percent yield is determined using the crude mass of the isolated addition product