Click Chemistry: The Thiol-Alkene Reaction

Chemistry so easy, even a physicist could do it!

-Charles Hoyle

2nd & 4th block Chemistry
How many shoes would a spider need?

You automatically say 8, but here’s the process that you’re going through:

• 1 spider has 8 feet
• 1 foot fits into 1 shoe

\[
\begin{array}{ccc}
1 \text{ spider} & 8 \text{ feet} & 1 \text{ shoe} \\
1 & 1 \text{ spider} & 1 \text{ foot}
\end{array}
\]

= 8 shoes
Stoichiometry Review

How about a mole of spiders?

- $6.02 \times 10^{23}$ spiders
- 1 spider has 8 feet
- 1 foot fits into 1 shoe

\[
\frac{6.02 \times 10^{23} \text{ spiders}}{1 \text{ spider}} \times \frac{8 \text{ feet}}{1 \text{ foot}} = 4.8 \times 10^{24} \text{ shoes}
\]

Compare this equation with the one that we used on Slide 2:

\[
\frac{1 \text{ spider}}{1 \text{ spider}} \times \frac{8 \text{ feet}}{1 \text{ foot}} = 8 \text{ shoes}
\]
Vocabulary

- **Thiol** – a molecule containing at least one sulfur-hydrogen single bond
  - Thiols give skunk spray its smell
- **Alkene** – a molecule containing at least one carbon-carbon double bond
- **Photoinitiator** – a molecule that starts a reaction in the presence of light
- **Functionality** – the number of reacting groups in a molecule
How the Photoinitiator Works

The PI is activated by light with a wavelength of 365 nm.

**Question:** What is a good source of ultraviolet light?

<table>
<thead>
<tr>
<th>Color</th>
<th>Peak Wavelength [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blue</td>
<td>470</td>
</tr>
<tr>
<td>Cyan</td>
<td>525</td>
</tr>
<tr>
<td>Green</td>
<td>560</td>
</tr>
<tr>
<td>Yellow</td>
<td>585</td>
</tr>
<tr>
<td>Orange</td>
<td>600</td>
</tr>
<tr>
<td>Red</td>
<td>645</td>
</tr>
<tr>
<td>Deep Red</td>
<td>700</td>
</tr>
</tbody>
</table>
Click Reactions

- A click reaction must satisfy the following:
  - The reaction must be **fast**
  - The reaction must be **exothermic**
  - The reaction must result in a **high yield of the desired product**
  - The desired product must be **easily separated**
  - The reaction can be run at or near **ambient conditions**
Thiol-Alkene Stoichiometry

Let’s consider a **monofunctional thiol** and a **monofunctional alkene**.

If we start with 10 g of **alkene**, how much **thiol** do we need for complete reaction?

![Reaction diagram](image)

1-hexene  
84.16 g/mol  
Thioglycerol  
108.16 g/mol  
The product is called a **thioether**.

**Questions:** Based on the product structure, how many thiols react with one alkene?  
What are the functionalities of 1-hexene and thioglycerol?
Thiol-Alkene Stoichiometry

Here’s what we’ve just seen:

- 10 g alkene
- 84.16 g alkene = 1 mol alkene
- 1 mol alkene = 1 mol C=C bonds
- 1 mol C=C bonds = 1 mol S-H bonds
- 1 mol S-H bonds = 1 mol thiol
- 1 mol thiol = 108.16 g thiol

These conversion factors are important, even though it’s just a whole bunch of ones.

12.85 g thiol
A Closer Look at the Equation

Starting amount of alkene molecule.

- **10 g alkene**
- **1 mol alkene**
- **84.16 g alkene**

Functionality of the alkene molecule

- **1 mol C=C bonds**
- **1 mol alkene**
- **1 mol C=C bonds**

Functionality of the thiol molecule

- **1 mol S-H bonds**
- **1 mol thiol**
- **1 mol S-H bonds**

Molecular weight of alkene molecule.

- **108.16 g thiol**
- **1 mol thiol**

Stoichiometry of thiol groups to alkene groups. This stays CONSTANT.

Molecular weight of thiol molecule.
Lab: The Thiol-Alkene Reaction

Let’s use a **trifunctional alkene** and a **tetrafunctional thiol**. Start with 10 g of trifunctional alkene. How much thiol do we need?

![Chemical structures](image)

- 10 g **trialkene**
- 256 g **trialkene** = 1 mol **trialkene**
- 1 mol **trialkene** = 3 mol **C=C bonds**

<table>
<thead>
<tr>
<th>10 g <strong>trialkene</strong></th>
<th>1 mol <strong>trialkene</strong></th>
<th>3 mol <strong>C=C bonds</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>256 g <strong>trialkene</strong></td>
<td>1 mol <strong>trialkene</strong></td>
</tr>
</tbody>
</table>

- 1 mol **C=C bonds** = 1 mol **S-H bonds**
- 4 mol **S-H bonds** = 1 mol **tetrathiol**
- 1 mol **tetrathiol** = 489 g

<table>
<thead>
<tr>
<th>1 mol <strong>C=C bonds</strong></th>
<th>1 mol <strong>S-H bonds</strong></th>
<th>1 mol <strong>tetrathiol</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>1</td>
</tr>
</tbody>
</table>

14.3 g **tetrathiol**
Thiol-Alkyne Reaction (Mr. J’s research)

- **Alkyne** – any molecule with at least one carbon-carbon triple bond
- The thiol-alkyne reaction has stoichiometry of **2:1 thiol:alkyne**
- The product is called a **1,2-dithioether**
Thiol-Alkyne Reaction

- Given 10 g of a **difunctional alkyne** (222 g/mol), how much **trifunctional thiol** (399 g/mol) would be needed for a complete reaction?

\[
\begin{array}{c|c|c|c|c|c}
10 \text{ g dialkyne} & 1 \text{ mol dialkyne} & 2 \text{ mol CC bonds} & 2 \text{ mol S-H bonds} & 1 \text{ mol trithiol} & 399 \text{ g trithiol} \\
1 & 222 \text{ g dialkyne} & 1 \text{ mol dialkyne} & 1 \text{ mol CC bonds} & 3 \text{ mol S-H bonds} & 1 \text{ mol trithiol} \\
\end{array}
\]

24.0 g **trithiol**
Questions?

- Questions?
- Comments?
- Complaints?
- Desire to shout obscenities at the concept of stoichiometry?
- Tirades?
- Urges to throw something at Mr. Jungman?
- Riots?
- General consideration over the inwardly-contemplative-yet-outwardly-emotive state of mind?
- Praise?