Supplementary Information (SI) for RSC Sustainability.

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Case Study 2 - Greener Plastics: Addressing Single-Use Plastics
Week 1: Beginning-of-Life

Scenario:

Your team works as scientific advisors for your local congressperson. An NPR podcast has recently caused an uproar for your boss' constituency. The podcast highlighted the shortcomings of the current recycling programs for single-use plastics. The constituency is demanding action from the congressperson.

Understanding the limitations of their knowledge of the problem, the congressperson has tasked their scientific advisors (you and your group) to develop a **Policy Paper**. The paper should provide **background information on what plastics are**, the **scope of the plastic pollution problem**, and evidence used to argue in support of **one of two competing legislative proposals** (shown below):

1) Fixing problems associated with the **beginning-of-life (synthesis and sourcing)** of single-use plastic polymers.
2) Addressing problems with the **end-of-life (recycling/disposal)** of single-use plastic polymers.

Overall Goals for Case Study 2

During Case Study 2, your group will engage in a number of science and engineering practices using your knowledge of chemistry and the tools and data we have provided. Over the next four weeks, you will accomplish each of the following:

1. **Construct a molecular-level explanation of how and why** each polymer-forming reaction scheme occurs using your understanding of chemistry.
2. **Define the beginning-of-life problem** faced by the **polymer manufacturing** companies and **evaluate the strengths and weaknesses** to possible solutions to the problem.
3. **Define the end-of-life problem** faced by the **chemical recycling** companies and **evaluate the strengths and weaknesses** to possible solutions to the problem.
4. **Define the end-of-life problem** faced by the **chemical decomposition** companies and **evaluate the strengths and weaknesses** to possible solutions to the problem.
5. **Design a solution** to the congressperson's problem and communicate your group's solution through a **Policy Paper** that outlines an **evidence-based argument** of your choice of **which legislative proposal to support**.

Goals for Case Study 2 Week 1

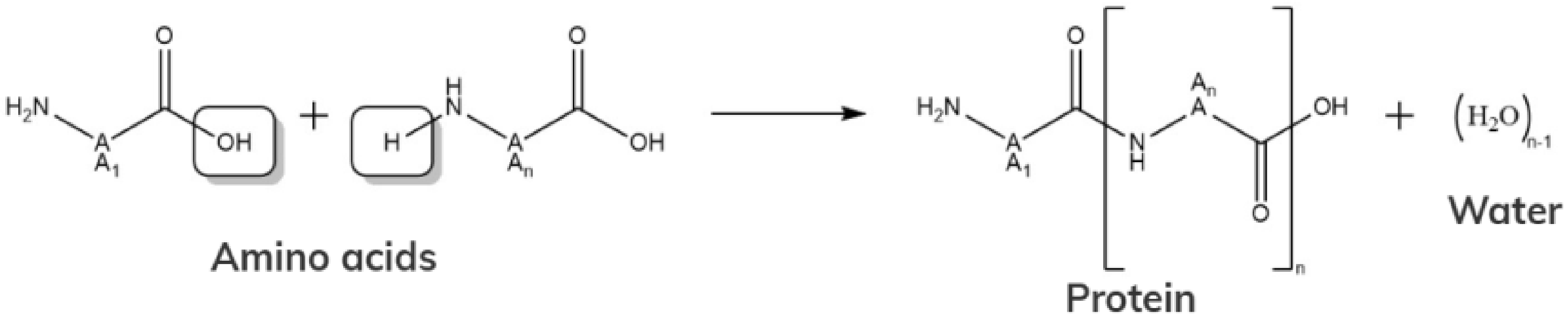
Constructing Mechanistic Explanations, Defining the Problem, and Evaluating Solutions

1. **Construct a molecular-level explanation of how and why** each polymer-forming reaction scheme occurs using your understanding of chemistry.
2. **Define the beginning-of-life problem** faced by the **polymer manufacturing** companies and **evaluate the strengths and weaknesses** to possible solutions to the problem.

One of the most common classes of polymers are "condensation" polymers. As the name suggests, water is removed from the monomer structure during the polymerization process.

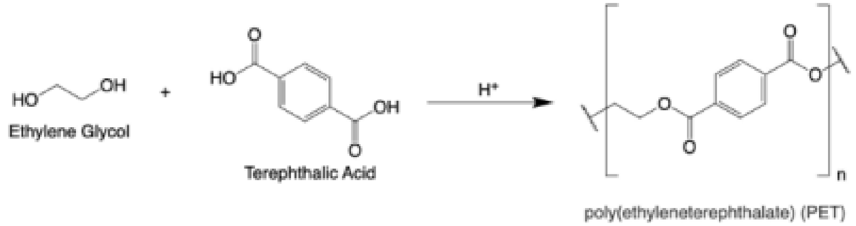
$$\text{Monomers} \xrightarrow{H_2O} \text{Polymer}$$

Examples from nature include proteins/polypeptides which can be classified as polyamides. Artificial polyamides include nylon.

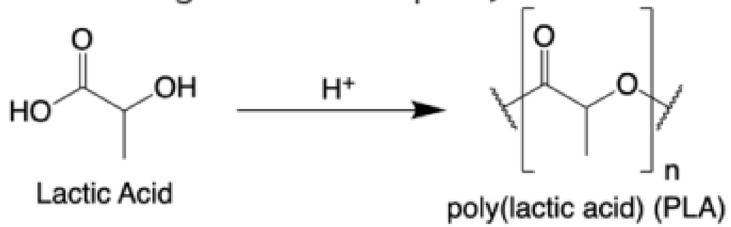


Polyesters are another major class of condensation polymers which are used in a wide range of industrial applications. One of their applications, that is a major contributor to the plastic waste problem, is their use in single use drink containers. The polymers focused on in this case study are traditionally used as disposable cups and bottles.

Traditionally, single use drink containers have been made of the condensation polymer poly(ethyleneterephthalate) (PET). PET is made by polymerizing two petrochemicals, ethylene glycol and terephthalic acid (shown below). The resulting polymer has many physical properties that make it suitable for the long-term storage of carbonated beverages.



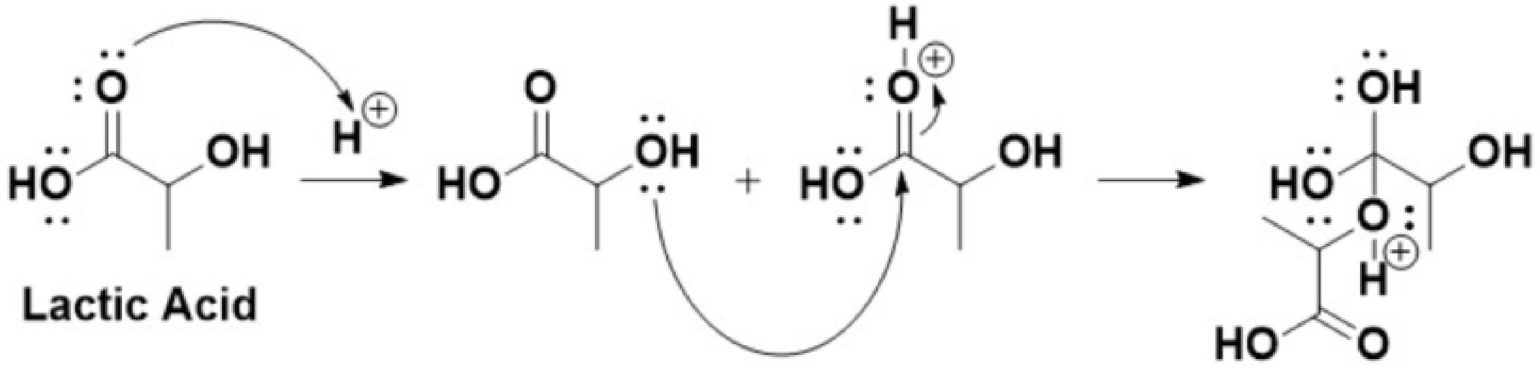
Recently, poly(lactic acid) (PLA) has emerged as an alternative to PET. PLAs building block, lactic acid, is sourced from plant material. The resulting polymer has physical properties comparable to those of PET, making it almost equally suitable for carbonated beverage storage.



This week, your group will be exploring the greenness and sustainability of making both polymers, PET and PLA. You will start by comparing the synthetic methods of each polymer and the impact of monomer sourcing.

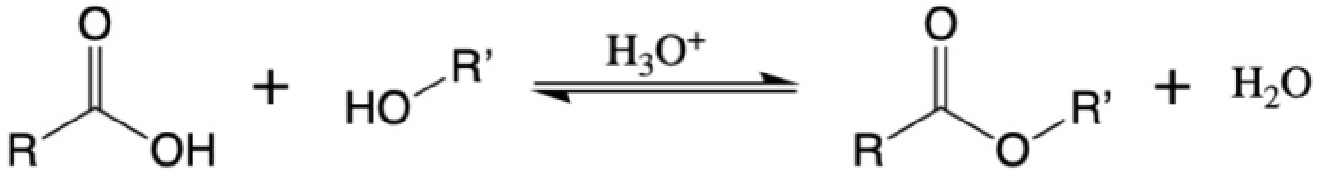
Acid Catalysis

These polymerization reaction are also known as **esterification reactions** since the product contains an ester functional group. There are usually a couple different ways to help promote formation of the products in these reactions. The first way this can be accomplished is by using an **acid catalyst**. The acid catalyst **activates the carbonyl** by making it **more electrophilic** and, thus, more susceptible to the nucleophilic attack an alcohol. Shown below are the first two steps of the **acid-catalyzed polymerization of Lactic Acid**. The **protonation of the carbonyl** (of the first Lactic Acid molecule) makes it **more electrophilic** for the subsequent **S_N2 reaction** in the second step when another Lactic Acid molecule "attacks" at the activated carbonyl -- also known as **"self-polymerization"**.



Shifting Equilibrium

Another way to help shift the equilibrium to the right towards the product is by **changing the concentration of either the reactants or products of the reaction**. For instance, if you remove one of the reactants of the reaction, the equilibrium will shift to the left to compensate for the missing reactant. You make recall that this phenomenon is described by **Le Chatelier's Principle**, which helps us predict the impact of a change in conditions on the equilibrium of the reaction.



In the esterification reaction shown above, **water is formed as a side product** to the reaction. If we **remove water** from this reaction as it is formed (continually decreasing the concentration of water), the system will respond by **shifting the equilibrium** towards the products to make up for this loss of water. Thus, **decreasing the concentration of water** also helps **speed up the rate of the forward reaction** and, thus, **shift the equilibrium to the right** towards the products.

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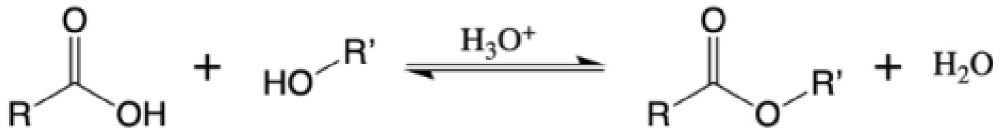
Because PET and PLA are both polyesters, their syntheses a very similar. Below is a table summarizing each synthesis. In the green box below, **suggest two methods** that these syntheses can use to **help shift equilibrium towards the products**. In your explanation, be sure to **describe the effect that each method would have on either reactants or products**. Hint: think about **the temperature at which water boils** and how this could be useful for one method.



Synthetic Detail	PET	PLA
Temperature (°C)	197	195-230
Solvent	None	None
Reaction Time (h)	3	2.5
Catalyst Used?	Yes	Yes
Special Glassware	Distillation Apparatus	None

Describe two methods to shift equilibrium to the products.

How Green and Sustainable Are These Reactions??

The Green Chemistry Behind PET and PLA Polymerization Reactions

As we have seen over the first part of this week's case study, the synthesis of PET and PLA are actually quite similar -- think acid catalysis and shifting equilibrium.

Now, let's look at these two reactions again, this time through the lens of Green Chemistry. How similar are these reactions in terms of their sustainability??

One method used to guide decision making in regards to green and sustainable chemistry are the 12 Principles of Green Chemistry. The following principles can be applied to the synthesis of PET and PLA. Would you consider the principle #5 (Safer Solvents and Auxiliaries: *The use of auxiliary substances (e.g. solvents, separation agents, etc.)* ***should be made unnecessary*** *whenever possible and innocuous when used* as a strength or weakness of synthesis? Explain your choice in the box below. Hint: refer back to the table on slide 9.

The principle, safer solvents and auxiliaries, is a ☐ Strength ☐ Weakness of the synthesis methods shown.

One method used to guide decision making in regards to green and sustainable chemistry are the 12 Principles of Green Chemistry. The following principles can be applied to the synthesis of PET and PLA. Would you consider the principle #6 (Design for Energy Efficiency: *Energy requirements of chemical processes should be recognized for their environmental and economic impacts and should be minimized. If possible, synthetic methods should be* ***conducted at ambient temperature (Room Temp) and pressure.****)* as a strength or weakness of synthesis? Explain your reasoning in the box below. Hint: refer back to the table on slide 9.

The principle, design for energy efficiency, is a
☐ Strength
☐ Weakness
of the synthesis methods shown.

Monomer Sourcing Data

Below is a table that describes the price and source of each of our monomers of interest. Keep in mind that there are many steps involved with getting monomers from the source to the companies that use them to make polymers. While there are a lot of beginning-of-life factors to consider in the life cycle of a chemical or chemical process, let's focus on analyzing the sourcing of each monomer.

Monomer	Price ($/ton)	Source
Ethylene Glycol	$33,570/ton	Petroleum
Terephthalic Acid	$29,540/ton	Petroleum
Lactic Acid	$40,900/ton	Sugar Cane (Plant Biomass)

There other factors about the monomer sourcing to consider, such as using a resource that could feed, shelter, or provide energy for homes. How does that impact the [UNESCO Sustainable Development Goals]() (UNSDGs)? Choose the 3 UNSDGs **(Blue Box)** that you feel will be the most impacted by monomer sourcing, predict how each UNSDG will be impacted **(positively/negatively - Multiple Choice box)**, and explain your prediction **(Green Box)**.

Impacted Sustainable Development Goal #1:

The UNSDG will be impacted ☐ Positively ☐ Negatively by a switch in monomer sourcing.

Explanation of Prediction:

Previous

Next

There other factors about the monomer sourcing to consider, such as using a resource that could feed, shelter, or provide energy for homes. How does that impact the UNESCO Sustainable Development Goals (UNSDGs)? Choose the 3 UNSDGs **(Blue Box)** that you feel will be the most impacted by monomer sourcing, predict how each UNSDG will be impacted **(positively/negatively - Multiple Choice box)**, and explain your prediction **(Green Box)**.

Impacted Sustainable Development Goal #2:

The UNSDG will be impacted ☐ Positively ☐ Negatively by a switch in monomer sourcing.

Explanation of Prediction:

Previous

Next

There other factors about the monomer sourcing to consider, such as using a resource that could feed, shelter, or provide energy for homes. How does that impact the UNESCO Sustainable Development Goals (UNSDGs)? Choose the 3 UNSDGs **(Blue Box)** that you feel will be the most impacted by monomer sourcing, predict how each UNSDG will be impacted **(positively/negatively - Multiple Choice box)**, and explain your prediction **(Green Box)**.

Impacted Sustainable Development Goal #3:

The UNSDG will be impacted ☐ Positively ☐ Negatively by a switch in monomer sourcing.

Explanation of Prediction:

Previous

Next

Defining the Problem

If we limit our analysis to just the industrial process of producing the polymer, we may find that one synthesis may be marginally greener than the other one. This limited view of the impact of chemistry on sustainability neglects all of the important chemical transformations, transportation of materials, associated costs, and the ethical/political implications of monomer sourcing (i.e., what is done to get the monomers to the chemical companies). Let's think about the problem of the beginning-of-life cycle of our monomers.

In the green box below, **describe the beginning-of-life problem with monomer sourcing** in Case Study 2 and **why it is a problem**. In your response, **identify the physical system** (in which the problem is embedded) and **its components**, **specify the stakeholders of interest** to the problem and match each stakeholder to the **criteria/constraints that are important** to consider when designing an acceptable solution.

Case Study 2 Week 1

List the **team names, MSU emails, and CEM section numbers** of everyone in your group who participated in this week's Case Study activity.

Leave this blank if you DO NOT intend to turn this in.

Team Member 1	MSU Email	Section Number
Team Member 2	MSU Email	Section Number
Team Member 3	MSU Email	Section Number
Team Member 4	MSU Email	Section Number

You must hit "Complete" to earn credit for the assignment.

Once you hit "Complete" your answers will be submitted to your instructor so make sure they reflect your final responses before hitting "Complete"