Waste and TinkerToys—Atom Economy

Objectives

1) Explore the idea of *atom economy,* or avoiding wastes by incorporating as much of the starting materials into the desired product as possible.
2) Relate the Law of Conservation of Matter to the idea of "wastes."
3) Discuss a "real world" application of atom economy.

Green Chemistry Principles

- Wastes? Why make them?
- It's midnight. Do you know where your product is?

IL State Standards (Science)

11.B.4a, 12.C.3b, 12.C.4b, 12.C.5a, 12.E.3c, 13.A.3a, 13.A.5a, 13.A.5c, 13.B.3a, 13.B.3c, 13.B.4b, 13.B.4d, 13.B.5b, 13.B.5e

Levels

Part 1: Middle school to high school.
Part 2: High school. Can be used in middle school with some modification.
Part 3: High school. Case study may be mentioned as example in middle school discussions of atom economy.

Vocabulary

Atom economy, percent yield, waste, formula weight, Law of Conservation of Matter, Life Cycle Analysis (LCA) [Include "LCA" as a vocabulary word if the suggested extension involving an LCA of a tennis shoe is used.]

Materials

One molecular model kit, TinkerToy set or equivalent per group of two

Time

One class period (May extend to additional class periods if suggested "Ideas for further study" are used.)

This material is adapted from the ACS text *Introduction to Green Chemistry.* See the "references" section of the introduction to this manual for additional information on this text.

Background/Overview

A main focus of green chemistry is to reduce the amount of pollution created in chemical processes. Reactions in which a large proportion of the reactant atoms end up in waste products contribute to pollution, make ineffective use of resources, and raise the costs of production. While percent yield is often considered a measure of how efficiently reactants are used in making a final product, it neglects to measure what fraction of the reactant atoms end up in the *desired* product. Atom economy, a concept introduced by Barry Trost of Stanford University, is a ratio that lets us know what percent of the reactants' atoms make their way into the desired product.

Part 1: What is a "waste" product? (Discussion)

Consider the following statement: A chemist suggests that it is impossible to "throw away" anything. The chemist goes on to say there is no such thing as "waste." Obviously, we dispose of many items in our everyday lives. What do you suppose this chemist means by saying says things *can't* be thrown away?

Questions & answers for Part 1: What is a "waste" product?

1. The Law of Conservation of Matter states "matter cannot be created or destroyed." How does this law relate to the statement made above by the chemist?

Atoms don't go away just because they have reacted, even though uninformed observations sometimes suggest this. When a candle burns, matter appears to be reduced and energy is given off. In fact, the matter simply turned into less observable gases and smoke.

2. Chemists sometimes refer to "byproducts" rather than "waste." What are some advantages and disadvantages of using such a term? List one of each.

A byproduct is still a product, so it helps reinforce the idea that "other stuff" was produced and needs to be considered. A disadvantage is that the term byproduct may suggest that it is useful, when it may not be.

3. On average, you have a couple of atoms in your body that were once found in the body of a dinosaur. Explain how this can be.

Atoms are continually recycled. A carbon atom that is part of your protein today will eventually be returned to the environment, where it will be incorporated in new compounds, perhaps in another living organism. Given the quantities of carbon atoms required to make a dinosaur and a human, it is statistically likely that some of your atoms were once used to make a dinosaur.

Instructional notes for Part 1: What is a "waste" product?

This activity is designed to reinforce the students' understanding of the Law of Conservation of Matter. All substances that we consider waste are made up of molecules and atoms that do not disappear just because we dispose of them. Things we label as waste and throw away because we have no use for them can be put out of sight and out of mind—but not out of existence. In a chemical reaction, atoms may end up as part of either the desired product or undesired byproducts.

It is good for students to realize that the number and kinds of atoms on earth are essentially fixed. A small amount of matter might leave the earth, a bit is gained from meteorites and such, and we have a limited amount of transmutation due to nuclear reactions. But other than that, what we have is what we have. Student misconceptions might arise from the observation of matter changing so profoundly in chemical reactions. Still, the fact is that chemical reactions only involve the making and breaking of bonds between atoms. The kind and total number of atoms remain essentially the same.

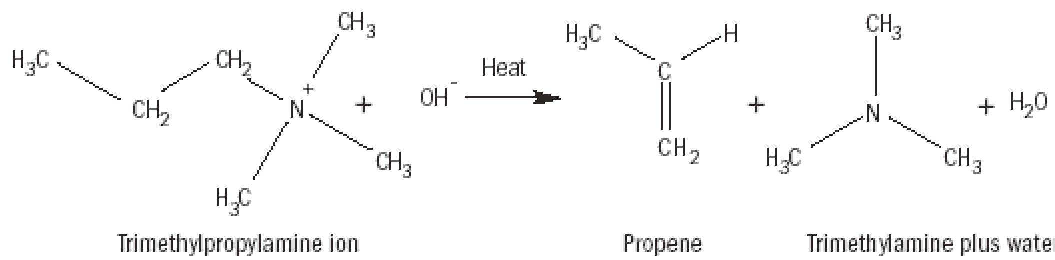
Part 2: Counting atoms—How can we calculate the atom economy of a simple chemical reaction? (Activity)

Chemists can build molecules by knowing the rules about how atoms combine. Chemical bonds being broken and new bonds forming can explain all chemical reactions. One simple organic molecule is propene, which is composed of three carbon atoms and six hydrogen atoms and has one double bond between two of the carbon atoms. There is more than one way to make propene. In this activity, you will consider two different reactions leading to propene and will use molecular model kits to investigate how the concept of atom economy can illustrate green chemistry.

Procedure

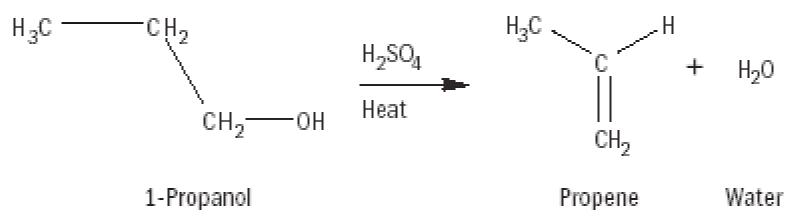
1) Use your molecular model kit (TinkerToys) to construct a trimethlypropyl amine ion. When this substance is heated, it decomposes into propene and two other products as shown below. Count the number of each kind of atom in the molecule.
2) "Heat" will be applied to your model and you will break it apart. Make one propene molecule. Place the rest of the atoms in a box marked "waste products." Count the number and kind of atoms in the propene molecule and the number and kind of atoms in the "waste box". When you are finished, dismantle your molecules.
3) Use your model kit to make a 1-propanol molecule. When this molecule is heated with a sulfuric acid catalyst, it also forms propene.
4) When your teacher indicates, break your molecule apart and make one propene molecule. Place the rest of the atoms in a box marked "waste products." Count the number and kind of atoms in the propene molecule and the number and kind of atoms in the "waste box." When you are finished, dismantle your molecules.

Reaction 1



vs

Reaction 2



Questions & answers for Part 2: Counting atoms

1. Compare the formula weight of the atoms in the waste box in reaction 1 to the formula weight of the atoms in the waste box in reaction 2. While this is not the way propene is produced on a mass scale, suppose reaction 1 were the conventional way of producing propene. What is the atom economy of this reaction?

Note: To quantify the concept of atom economy, we can calculate "percent atom economy". To do this, we divide the formula weight of the desired product by the formula weight of all the products of the reaction and multiply the result by 100. The calculation is displayed below:

$$\frac{\textbf{Formula weight of desired product}}{\textbf{Formula weight of all products}} \times 100 = \textbf{Percent atom economy}$$

Reaction 1: 42g desired product, 119g total of all products; atom economy = 35%
Reaction 2: 42g desired product, 60g total of all products; atom economy = 70%

2. What advantages would there be if reaction 2 were offered as a green chemistry alternative for the production of propene? What is the percent atom economy of this reaction?
Not only is the atom economy double in reaction 2, but the other product is simply water, a very benign byproduct.

Instructional notes for Part 2: Counting atoms

(*Note:* At the teacher's discretion, a standard percent yield experiment can be included in the activities of this module before this activity, if the teacher wishes to demonstrate that this is one familiar way of indicating the efficiency of a chemical reaction. The point should then be emphasized that percent yield generally is a comparison of actual yield of product compared to what was theoretically predicted from the balanced equation. The activity then introduces the concept of atom economy, which does account for the destination of the reactant atoms.)

In this activity, students are given two alternative procedures for producing a molecule. They use molecular model kits to make the desired molecule from specific reactants. After they break bonds from the reactants and make new bonds for the products, they are asked to sort the atoms into "waste products" and "desired products".

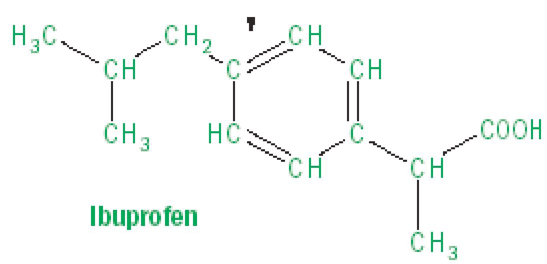
Students then calculate the atom economy for each reaction. If less waste is produced, it is an indication that the process might be more "green." Of course, a more acceptable atom economy is not sufficient on its own to make a process a good example of green chemistry. If the waste were more toxic than that which is produced in conventional processes, the reaction would be unacceptable.

Likewise, the new process has to make sense economically. Use whatever kind of molecular modeling kits you have available. You may have commercial model kits, TinkerToys, or alternatively, you can use gumdrops or other candies plus toothpicks to make the models. Any of these options will work well.

Part 3: Atom economy in the real world—Ibuprofen (Discussion)

In the Counting Atoms activity, you modeled chemical reactions and placed "unused" atoms into a "waste box." In chemical reactions, atoms that are not in the desired product are considered waste. This waste is analogous to the waste box in the previous activity. To make complex molecules (like the ones used in pharmaceuticals and pesticides), chemical engineers will often link together several reactions to form a chemical synthesis. Each step in the synthesis can be viewed as an individual reaction. As you saw in the Counting Atoms activity, atoms in a reaction can either end up in the final product or be discarded in a waste box.

Let's look at a common synthesis of ibuprofen (the active ingredient in the over-the-counter drugs Advil and Motrin, see below for its chemical structure). See the pages following this activity for the synthesis (Boots Co. synthesis from the 1960s)—you may display to your students on an overhead. The unused atoms during the synthesis are analogous to the atoms that you placed in the waste box in the Counting Atoms activity. In the early 1990s, the BHC Co. developed a new synthesis for ibuprofen (again, see the pages following this activity) that created far less waste because fewer atoms made their way into the waste box. Discussing this example with your students provides a "real world" connection for the concept of atom economy.



Ibuprofen

Atom economy is a useful concept for determining the efficiency of use of starting materials in reactions or syntheses. However, the presence of atom economy is not sufficient to consider a process "green." Some other important aspects of the process that must also be considered include:

- The nature of the waste produced: Is the waste toxic or environmentally harmful?
- The amount of energy needed to make the reaction proceed: Does the reaction require excessive amounts of energy?
- The use of auxiliary reagents: Does the synthesis require solvents or the use of significant amounts of materials to extract or purify the product?
- The percent yield of the reaction: Is a high yield of the product obtained, or is most of the desired product lost as waste?
- The selectivity of the reaction: Is the desired product produced in considerable preference to unwanted side products?

Ideas for further study

As an extension of your discussion about what a "waste" product is, students may benefit from considering what happens to the "waste" that we throw out each day. Where does "garbage" go in your community? Is there a local landfill, or is the waste transported to landfills elsewhere? What happens to materials once it is placed in a landfill? Do local recycling and composting programs exist? See the supplemental activities on solid waste and packaging that follow this activity for additional exercises that may be used as extensions of Part 1 of this exercise.

Another useful extension of the discussion of wastes is to perform a Life Cycle Analysis (LCA) of an everyday item. See the following Waste Management and Research Center (WMRC) fact sheet for an activity involving the LCA of a tennis shoe.

Finally, a great way to convey the idea of process efficiency to younger students is use a game as an analogy. One game that illustrates the imprtance of efficient processes graphically is the “peg game that is commonly found at Cracker Barrel restaurants. The object of this game is to move your pieces in such a way as to only have one peg remaining. If you don’t move efficiently, you’ll have additional pegs standing at the end of the game (which can be thought of as “wastes”) and you lose.

For more information on this game see the “toys” section of the Cracker Barrel’s online store at http://shop.crackerbarrel.com/online/, and look for “peg games.” (Note: This information is provided for reference only and should not be construed as an endorsement of Cracker Barrel by WMRC or any of the agencies involved with this workshop).

References

1. The U.S. EPA website (www.epa.gov/greenchemistry/aa98a.htm) provides more information on the concept of atom economy and on the Presidential Green Chemistry Challenge Award given to Barry Trost for his work on this concept.
2. For its new synthesis of ibuprofen, the BHC Co. received a 1997 Presidential Green Chemistry Challenge Award. A description of the award-winning work can be found at the U.S. EPA website at www.epa.gov/greenchemistry/aspa97.htm.
3. The following site provides additional information on ibuprofen and compares it with other pain-relieving drugs: www.yourhealth.com/ahl/2001.html.

This material is adapted form the ACS text Introduction to Green Chemistry.