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Exploring Green Chemistry Metrics with Interlocking Building Block Molecular Models

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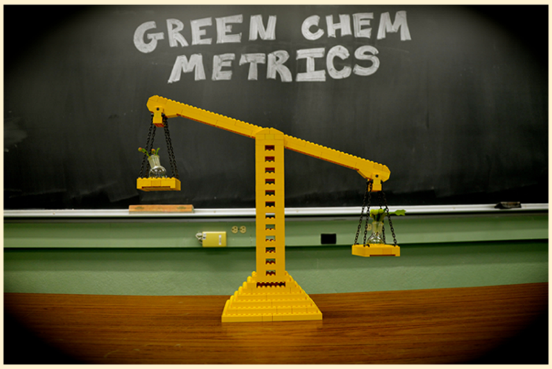
Supporting Information

ABSTRACT: A classroom activity for learning green chemistry metrics with interlocking building blocks is described. The activity illustrates the strengths and weaknesses of conversion, selectivity, yield, atom economy, reaction mass efficiency, carbon efficiency, E-factor, and effective mass yield by counting, where appropriate, the number of molecular models built, the number of bricks used, or the number of connection points available. The activity is appropriate for students in general chemistry courses through advanced undergraduate green chemistry or industrial chemistry courses.



KEYWORDS: *Green Chemistry, First-Year Undergraduate/General, Upper-Division Undergraduate, Analogies/Transfer, Organic Chemistry*

INTRODUCTION

Quantification of reaction efficiency with aims toward waste reduction continues to drive the development of new Green Chemistry metrics.[1,2] Where conversion represents the amount of starting material transformed, yield more specifically measures starting material converted into desired product and selectivity denotes the ratio of desired product to converted starting material. Developed by Barry Trost, and included by Anastas and Warner into their 12 Principles of Green Chemistry,[1,3] atom economy[4,5] addresses the theoretical amount of starting material incorporated into the final product. Many pericyclic reactions, for example, incorporate all atoms from the starting material into the final product (100% atom economical), whereas elimination reactions necessarily involve the loss of material. While atom economy measures theoretical starting material incorporation, it excludes consideration of yield and reagents in excess, which reaction mass efficiency addresses by including in the measurement of the actual mass of all starting materials and final products. Carbon efficiency excludes all other elements in a metric otherwise similar to reaction mass efficiency by only considering the amount of carbon in the starting material and product. Since solvents and auxiliaries represent important components of the waste stream, E-factor[6,7] measures the total waste for a given reaction. With the understanding that not all waste harms human health or the environment, effective mass yield essentially incorporates the essence of E-factor, but excludes benign reaction components, like water (Figure 1).

With much more material to cover in Green Chemistry or Industrial Chemistry courses, these metrics can be all too easy for instructors to present in a passive manner on a few simple slides or chalkboard equations. To offer opportunities for active learning,[8−10] this quick activity puts the starting materials and products in the hands of students in the form of interlocking building blocks and enables them to visually work through the strengths and weaknesses of various green chemistry metrics.

OVERVIEW

In this activity, students explore various reaction metrics through the assembly, alteration, and disassembly of interlocking building block[11−16] molecular models. Unlike conventional molecular modeling kits, interlocking building blocks provide the versatility to easily visualize not only entire molecules and individual atoms, but mass as well. With these blocks, a completed model represents a molecule, a brick represents an atom, and the number of connection points (both visible and covered) represents the molecular weight (Figure 2). Constructing and comparing visual representations of conversion, selectivity, yield, atom economy, reaction mass efficiency, carbon efficiency and E-factor helps students to understand the strengths and weaknesses of each metric.

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Conversion: $\frac{\text{converted starting material}}{\text{available starting material}} \times 100\%$

Selectivity: $\frac{\text{desired product}}{\text{converted starting material}} \times 100\%$

Yield: $\frac{\text{desired product}}{\text{available starting material}} \times 100\%$

Atom Economy: $\frac{\text{theoretical product mass}}{\text{theoretical starting material mass}} \times 100\%$

Reaction Mass Efficiency: $\frac{\text{actual product mass}}{\text{actual starting material mass}} \times 100\%$

Cartbon Efficiency: $\frac{\text{actual carbon in product}}{\text{actual carbon in starting materials}} \times 100\%$

E-factor: $\frac{\text{total waste (mass)}}{\text{total product}}$

Effective Mass yield: $\frac{\text{mass of products}}{\text{mass of non benign reagents}} \times 100\%$

Figure 1. Green chemistry metrics.

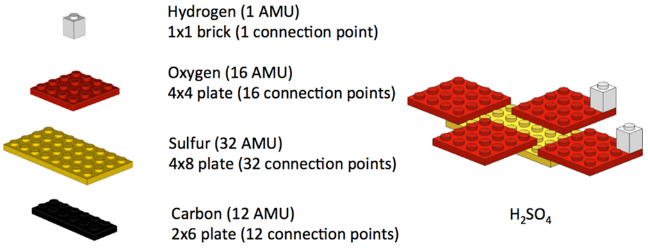

Figure 2. Representation of molecules, mass, and atoms with interlocking building blocks.

■ AUDIENCE

While the content of this activity is most suitable for students in an undergraduate green chemistry or industrial chemistry course, the baseline chemical knowledge needed to comprehend the material is quite fundamental, so even students in a college or high school general chemistry course can gain from the activity.

We ran this activity with a group of 10 prematriculation students in a green chemistry module and found that their high school chemistry training was enough for them to complete the exercise, having learned that the various metrics provide different quantifications of waste and resource utilization. These prematriculation students tended to tally the molecular composition of each compound, represent it primarily as a formula on paper from then on and to use the bricks/models only at the end to visually represent what they had already worked out on paper. The upper-level Green Chemistry audience, with a background in organic chemistry, could better conceptualize the retention of chemical complexity (represented as connected bricks) in places and the transformation of functional groups in other places, so the models themselves served as the primary tool for working through each metric. This exercise allows instructors to slow their descriptions of formulas and metrics, enabling students to visualize what each includes and what each leaves out. In both the prematriculation and upper level course, students worked in pairs or small groups on a single metric and successfully explained to the class (a) how they arrived at their visual representation, (b) what their metric considered/left out, and (c) the merits and weaknesses of their metric relative to others.

Since this activity uses the number of connection points as a representation for mass, it has the potential to conflate *atomic size/radius* with *molecular weight*. Therefore, instructors should note that the size/area of a brick scales with molecular weight rather than the actual size/radius of the atom it represents. We acknowledge the potential for a mix-up, but our students have not yet expressed this confusion, because the exercise does not consider atomic radius. Rather than ponder the representation of mass through spatial dimensions, students do question the difference in the vertical dimension of hydrogen (thicker bricks) versus other atoms (thinner plates), but those who grew up playing with these blocks invariably chime in to lament the difficulty of separating a thin 1 × 1 plate from a larger plate without resorting to the use of teeth or long finger nails; a taller 1 × 1 brick provides an easier handle for separation. We chose not to use thicker bricks for the other atoms to save considerable space and money.

This activity adds to the growing number of green chemistry[17,18] themed activities,[19] demonstrations,[20] and laboratory exercises[21] suitable for students at or below the advanced undergraduate level.

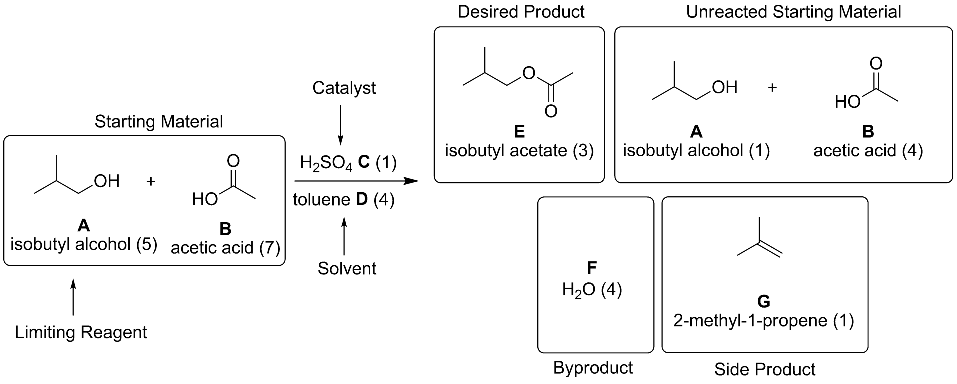

Figure 3. Acylation of isobutanol with interlocking building block molecular models. Parenthetical numbers indicate the moles/models/molecules for each compound at the start and finish of the reaction.

ACTIVITY DETAILS

The Supporting Information contains detailed step-by-step color guides for the construction of each reagent and product in the acylation of isobutanol. We provide two sets of materials lists. The first is for instructors on a tighter budget, which requires students to represent the various metrics one at a time with a single set of blocks. Students either assemble or receive preassembled models for the reagents, solvent, catalyst, desired product, unreacted starting material, byproduct and side product in the amount indicated in Figure 3. In this acylation of isobutyl alcohol, the alcohol is the limiting reagent with 5 models. Three are converted to the desired isobutyl acetate, one is converted to 2-methyl-1-propene, and one is left unreacted. Water is produced as a byproduct, and the excess acetic acid is left unreacted.

Students are asked to represent calculations of the various metrics using either entire models, individual bricks, or by the number of connection points. The various metrics can be represented as described in Table 1. An explanatory video, which can be used for reference, or shown in lieu of the activity, is available in the Supporting Information.

Table 1. Interlocking Building Block Representation of Various Metrics To Evaluate the Acylation of Isobutanol

Metric	Representation
Conversion	(3 models (**E**) + 1 model (**G**))/5 models (**A**)
Selectivity	3 models (**E**)/(3 models (**E**) + 1 model (**G**))
Yield	3 models (**E**)/5 models (**E**)
Atom Economy	no. of connection points in 1 **E**/(no. of connection points in 1 **A** + 1 **B**)
Reaction Mass Efficiency	no. of connection points in 3 **E**/(no. of connection points in 5 **A** + 7 **B**)
Carbon Efficiency	no. of carbon bricks in 3 **E**/(no. of carbon bricks in 5 **A** + 7 **B**)
E-factor	(no. of connection points in 1 **A** + 4 **B** + 4 **F** + 1 **G** + 1 **C** + 4 **D**)/no. of connection points in 3 **E**
Effective Mass Yield	no. of connection points in 3 **E**/(no. of connection points in 1 **A** + 4 **B** + 1 **G** + 1 **C** + 4 **D**)

DISCUSSION

Upon completing their molecular model interlocking building block representation of various green chemistry metrics, students should be able to explain which reaction components receive consideration in which metrics and whether the metric requires the number of molecules/moles (represented by a completed model), the number of atoms (represented by an individual brick), or instead the mass (represented by the number of connection points), whether theoretical (in the case of atom economy) or actual (in the case of reaction mass efficiency, E-factor, and effective mass yield). More importantly, students should be able to compare the merits and shortcomings of each metric, and decide for themselves when applying certain metrics is useful.

CONSIDERATIONS FOR ALTERNATIVE REACTIONS

Given the versatility of interlocking building blocks, instructors can design their own reaction to compare the various metrics. Since the geometry of commonly available building blocks limits the number of representable atoms, we chose the acylation of isobutanol as the reaction for this activity because it requires only hydrogen (1 × 1), carbon (2 × 6), oxygen (4 × 4), and sulfur (4 × 8). Certain other important atoms otherwise unrepresentable with commercially available bricks can be achieved with some modifications (Supporting Information). Though 2 × 7 bricks are not commonly sold, nitrogen (14 AMU) can be made by cutting one row (2 × 1) off a 2 × 8 brick. Similarly, fluorine (19 AMU), chlorine (35 AMU), and boron (11 AMU) can all be made by cutting a 1 × 1 square from the corner of a 2 × 10, 6 × 6, or 2 × 6 brick, respectively (SI Figure 1). Rather than sawing bricks, instructors can create the noncommercially available bricks by gluing together small pieces (SI Figure 2). Instructors should consider the limitations and potential fixes for commercially available bricks if they chose to use their own reaction for this activity. If designing their own reaction, instructors should, in addition to the limitation of representable bricks, consider the following:

1. Leave some starting material unreacted to differentiate conversion from other metrics.
2. Generate a side product to illustrate selectivity.
3. Use a catalyst and/or solvent for consideration in E-factor and effective mass yield.
4. Have a limiting and excess reagent to differentiate the theoretical mass used in atom economy from the actual mass in reaction mass efficiency, E-factor and effective mass yield.

Finding a reaction that can be represented by commercially available bricks and satisfies all these additional criteria can be difficult, so instructors may need to make some concessions. For example, in the acylation reaction described herein, it is unlikely that the elimination side product **G** would form in any appreciable quantity, though to avoid using the number of bricks (and student/instructor time) that it would take to build enough desired product **E** to make the proportions more realistic, we instead suspend our disbelief over the unrealistic proportions in order to better illustrate the differences between the various metrics. Similar concessions may need to be made for self-designed reactions as well.

ASSOCIATED CONTENT

Ⓢ Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.5b00696.

Detailed materials lists (PDF, DOCX)
Visual assembly instructions (PDF)
Explanatory video (ZIP)

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Notes

The authors declare no competing financial interest.

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