CHEM 489 Advanced Environmental Chemistry – Spring 2020

WORKSHEET #1 ANSWER KEY

Worksheet #1: Read PDF articles 1-4 found on the course web page, and review the 12 Principles of Green Chemistry (handout). These articles provide a good overview of green chemistry, are an easy read, and may be helpful in answering some of these questions. You should answer these questions on a separate sheet of paper. You can work together, but must submit your own worksheet and your own answers.

1. Define green and sustainable chemistry (in your own words please).
Any of the following would be accepted:

Technical. Green Chemistry aims to reduce or eliminate the use and generation of hazardous substances associated with the design, manufacture, and use of chemicals.

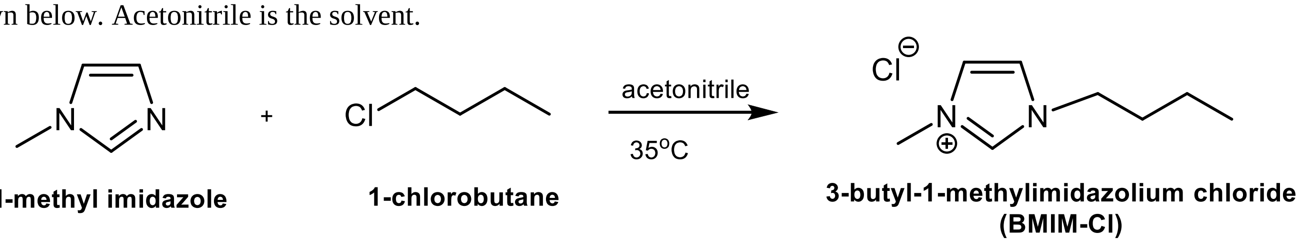
Molecular Design. Green chemistry is an approach to chemistry that aims to maximize efficiency and minimize hazardous effects on human health and the environment. This can be accomplished by implementing the 12 Principles of Green Chemistry.

Risk Assessment. Risk = Hazard x Exposure x Vulnerability

2. In your own words, give you opinion on how green chemistry and sustainability are or are not related.
This is an open-ended question where you could argue either way. Based on class lectures you might have addressed this question as: Green chemistry prevents pollution at the source by using innovative chemical processes to provide society with the products on which it depends. Green chemistry principles minimize the use of materials that are hazardous to human health and the environment, decreases energy and water usage, and maximizes efficiency. Thus, green chemistry has the potential to solve critical global challenges as climate change, sustainable agriculture, energy, toxics in the environment, and the depletion of natural resources.

3. What is the purpose of the 12 Principles of Green Chemistry?
The 12 Principles are both a set of guidelines for the design and invention of the next generation of materials needed by our society and economy, using processes that will have minimal adverse consequences to human health and the environment. By applying the 12 Principles of Green Chemistry, it becomes possible to achieve the synergism of economy, social justice, and environment by working at the molecular level.

4. Simple application of Green Chemistry Principles. A student synthesized the ionic liquid BMIM-Cl using the reaction shown below. Acetonitrile is the solvent.



(a) From this list, identify the type of reaction, and explain your answer: SN1, SN2, E1, E2, Electrophilic Addition
SN2 substitution reaction as a nucleophile (N-methyl imidazole) substitutes for the primary Cl leaving group.

(b) Define % Yield and % Atom Economy. How do these two metrics differ?
We use % yield and % atom economy as metrics to evaluate the efficiency of a chemical reaction or process. The ideal atom economy (100% atom economy) is where all reactant atoms are incorporated in the desired product. Atom economy is calculated by comparing the molecular mass (atoms) of the desired product to the sum of the molecular masses (atoms) of all reactants. A balanced chemical equation is required, as are stoichiometric multipliers for molecular mass. Atom economy takes into account how efficiently all the reactant atoms are used in a reaction. The higher the atom economy the lower the amount of waste produced.

The % yield is calculated by comparing the moles (mass) of the limiting reactant to the moles (mass) of the desired product(s). % Yield does not take into account the amount of waste produced.

(c) Do all reactant atoms end up in the desired product? If no, which atoms do not? Without doing a calculation, what is your preliminary assessment of the reactions Atom Economy?
Yes, all reactant atoms end up in the product, so we have 100% atom economy.

(d) Based on the balanced equation given above, what component(s) of this reaction is/are not considered in evaluating efficiency based on % Yield and Atom Economy?
The energy used for running this reaction at 35ºC, and the solvent, acetonitrile.

(e) Based on your lab experience (especially CHEM 243/244 labs), what other components of this process might be relevant to a full assessment based on Molecular Design?
Any additional solvents for workup, use of water for washing, etc., and drying agents are not considered. All these would contribute to the waste from this process.

(f) This reaction used 5.0 g of N-methylimidazole and 20.0 g of 1-chlorobutane. Loo up or calculate the molecular weight and number of moles of each. Based on the stoichiometry in the balanced equation, do you see a potential problem here? Explain.

MW of N-methylimidazole = 82.10 g/mole   MW of 1-chlorobutane = 92.57 g/mole
5.0 g of N-methylimidazole = 0.061 mole   20.0 g of 1-chlorobutane = 0.216 mole
The reaction stoichiometry is 1:1, but there is an excess of 1-chlorobutane. The excess of 1-chlorobutane will end up as waste unless it can be recycled and reused.

(5) Compare and contrast how green chemists reduce Risk as compared to traditional "command and control"?
Risk is a function of the Hazard, Exposure and Vulnerability; Risk = f(Hazard x Exposure x Vulnerability). Establishing environmental laws attempts to reduce Risk through "Command & Control," or Treatment & Abatement; in other words trying to control the problem after the fact. Green Chemistry reduces Risk by reducing or eliminating the Hazard, so protection from Exposure is unnecessary, those most vulnerable are less affected, and Command & Control Regulations (and their inherent costs) are not necessary.

(6) The 12 Principles of Green Chemistry can serve as a useful guide to the design, creation and use of chemicals and chemical technologies focused on the potential for human health and environmental benefits. For each idea or concept in the table below, identify a Primary and Secondary green chemistry principle that might apply. You do not need to justify your answers.

The answers here can be subjective and depend on the interpretation of the Principles by the user!

Idea or Concept	Application of 12 Principles of Green Chemistry	
	Primary	**Secondary**
Simplifying the overall process by reducing the number of steps	**1,6,8,12**	
Reducing the need for solvents and reagents and their risks	**5**	**1,3,8,12**
Reducing energy use for heating, drying and/or cooling	**6**	**7,8,9**
Use of safer processes and chemicals	**3,4**	**1,5,8,10,11,12**
Processes based on aqueous solutions instead of organic solvents	**5**	**1,3,10,12**
Developing more efficient processes that minimize waste	**1,2**	**3,4,5,8,10,12**
Continuous process production with real time monitoring and control	**11**	**1,4,6**
Recycling chemicals used in the process	**1**	**5,9**
Production and use of biodiesel as fuel	**7**	**10**
Plastics made from plant products rather than crude oil fractions	**7**	**3,4,10**
Development and use of solar, geothermal, wave or wind energy	**6**	**1,7**