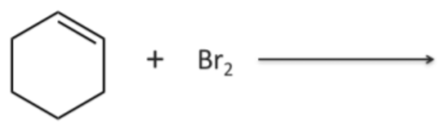
6.4: Conclusions and Review

In this final chapter, we became very familiar with the concepts of reaction efficiency and design from a green chemistry perspective. We more or less employed the totality of the green chemistry principles to understanding what goes into maximizing the environmental, social, and economic benefits associated with scientific enterprises. We thoroughly explored the nature of the various types of reactions done in both fundamental and applied settings and how to evaluate them using very useful mathematical constructs. This chapter serves to cement the concepts we learned in this magnificent discipline and to provide a platform for understanding how to best approach the chemistry, chemical engineering, and the biological transformations of reactions and processes.

Review Questions

1. Indicate by drawings what the addition products are for the following reaction and what type of reaction it is:

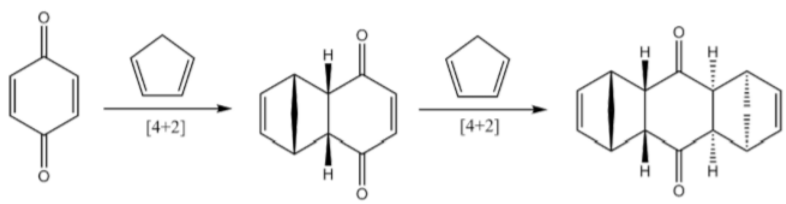


2. Please indicate what the products are of the reaction of 2-phenyl isopropyl iodide with sodium methoxide.

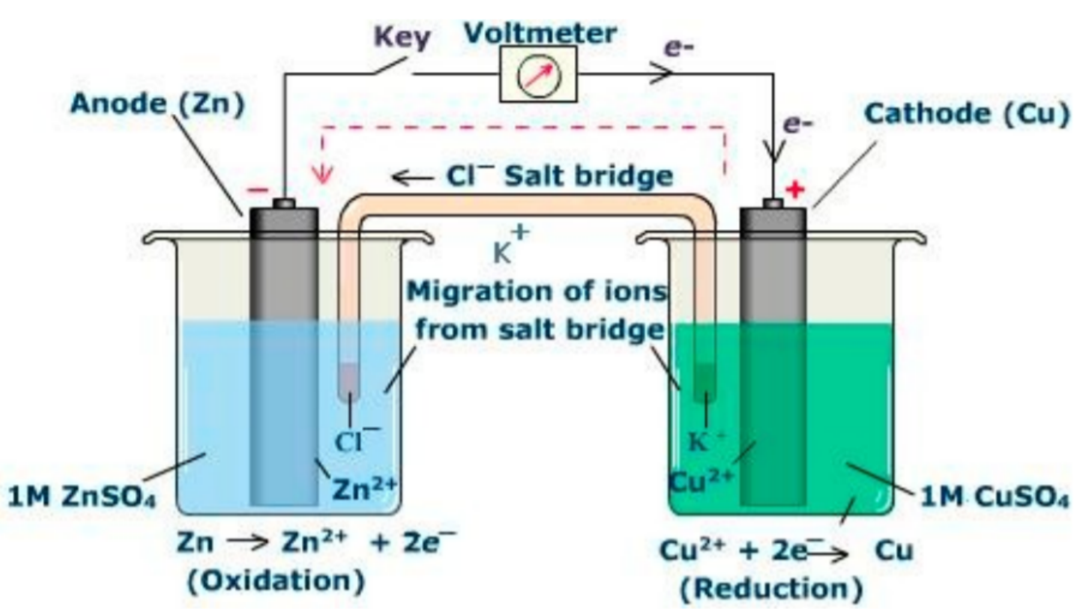
3. Does the non-salt product in (2) retain its stereochemical configuration? Why?

4. Please explain how the minor product is formed in the E2 reaction below and why it is minor?

5. Using the Diels-Alder Reaction shown below, draw the transition state that will lead to the adduct.



6. Using the redox diagram below, indicate why the process cannot go on forever



7. Define the following terms

a. atom economy

b. percent atom economy

c. percent yield

d. percent experimental atom economy

e. percent atom economy x experimental atom economy

8. Which of the terms in question 7 are only meaningful with experimental results? What experimental result is necessary to make these terms meaningful?

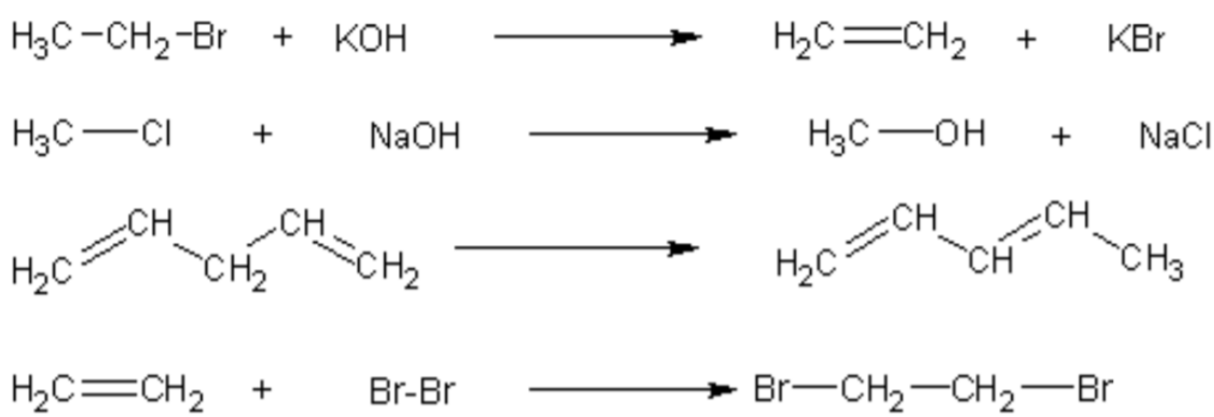
9. Consider the following four (4) reactions shown below:

a. Label each reaction as a substitution, elimination, addition or rearrangement.

b. Rewrite each reaction making sure that the reaction is balanced. Show all the reactant atoms that are incorporated into the desired product, and the atoms of the desired product in green, and all other atoms in brown.

c. Set up a table of atom economy whose headings are: formula, formula weight, number of utilized atoms, weight of utilized atoms, unutilized atoms, and weight of unutilized atoms.

d. Calculate the %-atom economy of each reaction



10. In the Further Reading section (#3), Roger Sheldon has developed a term very similar to the %-atom economy termed % atom utilization. The % atom utilization can be calculated according to the following equation: % Atom Utilization = (MW of desired product/MW of all products) X 100

a. Compare and contrast this with the %-atom economy

b. What concept that you learned in freshman chemistry makes the actual percentages calculated for the % atom utilization, and % atom economy equal (in most circumstances). Prove this by calculating the % atom utilization for each of the reactions in questions 9—13 and comparing your results to the %-atom economy that you calculated in question 9.

Further Reading

1. Williamson, Kenneth L., Macroscale and Microscale Organic Experiments, 2nd ed., D. C. Heath and Co., 1994, 247-252.
2. Trost, Barry M., The Atom Economy-A Search for Synthetic Efficiency. Science 1991, 254, 1471-1477.
3. Cann, Michael C.; Connelly, Marc E. Real-World Cases in Green Chemistry; ACS, Washington, 2000. Roger Sheldon of Delft University has developed a very similar concept called % atom utilization. Sheldon, Roger A. Organic Synthesis- Past, Present and Future. Chem. Ind. (London), 1992, (Dec), 903-906.
4. Anastas, Paul T., and Warner, John C. Green Chemistry Theory and Practice, Oxford University Press, New York, 1998.
5. Westheimer, T. The Award Goes to BHC. Chem. Eng. 1993, (Dec.), 84-95