

## STRUCTURE-REACTIVITY RELATIONSHIPS: HYDROCARBON REACTIVITY

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### INTRODUCTION

This experiment is an investigation of chemical reactivity. Remember that science is about discovery, it is about investigating and finding out things that you don't really know much about and testing theories. However, sometimes things don't go according to plan and maybe then learning something new or it reveals the need for further work. Since chemistry is a practical experimental science, it is about planning and carrying out experiments and making observations that you then try to rationalise and explain in order to learn something that can be applied to other situations. This experiment normally requires careful experimental work, making good observations then careful analysis of the results to deduce information about the systems being studied. Since we are online, there is a presentation including a video that you will need to watch to make your observations *etc.*

The experiment investigates the reactivity of some representative hydrocarbons towards the halogen bromine. It's a guided inquiry activity. Despite the fact that the answers to the questions that this experiment investigates are known in the scientific literature, there are aspects that may not be known to you (yet), and therefore, as far as you are concerned, this is a "*research*" activity. One of the aims of the experiment is to help you develop better problem solving skills as you analyse the results and learn something from laboratory work.

Remember that chemistry is about molecules and their properties. Chemists want to know what happens (and why) at the molecular level (e.g. reaction mechanisms) : they are molecular engineers. Recall that molecular structure controls the function - the properties of that compound. This experiment is also an example of what can be described as a "structure - activity relationship" investigation.

As you should know from lectures, in general, hydrocarbons and especially alkanes, are fairly unreactive because they lack polar bonds since they only contain C and H atoms which have very similar electronegativities. However, hydrocarbons are very important as chemical "feedstocks" (*i.e.* raw materials) as they are readily available from crude oil and they can be converted into other molecules containing more reactive functional groups, e.g. alkyl halides and then alcohols.

You will be studying the reaction of a series of hydrocarbons : toluene, ethylbenzene, isopropylbenzene, t-butylbenzene, cyclohexane and cyclohexene, with bromine in order to assess the relative reactivity of these systems by observing how the colour of the solutions change. **Note that bromine is a dark red or brown liquid whereas most simple hydrocarbons and alkyl halides are**

**colourless.** In your report, you will need to interpret the observed relative rates in terms of the structure the hydrocarbon substrate - **in order to do this you will likely need to do some background research on the reactions of hydrocarbons with bromine** - use the references provided as a starting point. We suggest you start to work on the report template before the laboratory period. You should have completed parts 1-4 before the laboratory session.

The report template is structured to help guide you through the process of result analysis and reaching conclusions.

**Remember, science is about making careful observations based on good experimental technique and then interpreting and explaining your results. That means you don't always know the answer or the theory before you carry out the experiment. In this case, carefully working through the results, asking good, appropriate questions and thinking, applying important chemical principles should allow you to rationalise the results.**

Here are some concepts that will help you with your analysis.

1. The important chemical principle that structure determines function. In this experiment, that will mean differences in structure dictate or control differences in the observed reactivity.
2. Look at the differences in structures to help explain the differences in reactivity.
3. When making comparisons, try to minimise the differences in the structures, so look for pairs that are similar. If there are too many differences, then you can't tell what factor is causing the difference in reactivity.

## **REFERENCES**

1. a. M. Jones and S. A. Fleming, in "Organic Chemistry", Norton: 4<sup>th</sup> edn., Chapter 11, pp. 468-81, 490-500 Chapter 10, pp. 409-20, Chapter 13, pp. 610-13, Chapter 14, pp. 631-9.  
b. M. Jones and S. A. Fleming, in "Organic Chemistry", Norton: 5<sup>th</sup> edn., Chapter 12, pp. 545-59, 568-78 Chapter 11, pp. 488-97, Chapter 14, pp. 678-81, Chapter 15, pp. 698-705.

<http://www.chem.ucalgary.ca/courses/351/Carey5th/Ch04/ch4-4-4.html>

<http://www.chem.ucalgary.ca/courses/351/Carey5th/Ch06/ch6-7.html>

<http://www.chem.ucalgary.ca/courses/351/Carey5th/Ch12/ch12-5.html>

## **REPORT**

Before writing any Chem 351 laboratory report, we strongly recommend that you review section 8 in the introductory section of the [student laboratory manual](#) that discusses how to write reports and/or from "[writing reports](#)" on the course website. Students often don't get the grades they would like because they make errors that are addressed in that section of the manual. These are avoidable errors.

Remember that more is not necessarily better. It is important to be accurate and concise rather than verbose and vague. Proper English should be used and it should be written in your own words.