Chemistry 3LI3
Chemistry Laboratory Inquiry

Course Outline Spring 2006

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Introduction

Chemistry is an experimental science. We develop concepts of what holds molecules together and how they react, but these are all tested and developed in the laboratory. Interesting and challenging labs are an essential part of the chemistry curriculum. Chemistry 3LI3 is an inquiry course that is focussed on experimental work, without being restricted to any particular type of chemistry. In particular, material from previous courses is combined and integrated. As in any inquiry course, students are expected to take an active role in the teaching and learning.

This course is intended to be a bridge between the standard one-afternoon undergraduate laboratory and the long-term research program you will encounter in Chemistry 4G06 (the senior thesis course). There are no formal lectures involved, but there will be occasional lectures to cover some of the material. There are two afternoons in the laboratory. There will be a number of basic experiments that everyone will do, but then there will be freedom to go deeper into some of the methods involved. You will also be encouraged to use (and understand) advanced equipment, such as FT-NMR, GC-MS, capillary electrophoresis, etc. This is a relatively new type of course for the Department, so the course details may change as the term develops. In 2006/07, Dr. Vargas-Baca will take over this course, so the details may change. However, the approach of "not your standard chemistry lab" will remain.

The next pages take you through an example of one of the experiments.

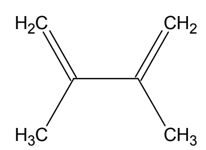
Evaluation

There will be three presentations during the term. The first one (in the week of January 17/18) will not count for marks, but the other two will. Assignments (3-4) on specific topics will be handed out. The lab performance mark will be an overall score judged by the TA's. There will be no final examination, but there will be a substantial term test (scheduled for 2-3 hours) towards the end of the term. The breakdown of marks will be as follows:

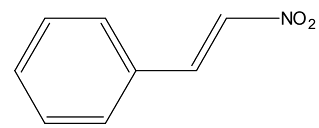
Presentations	15%
Assignments	15%
Lab reports	25%
Lab performance	10%
Midterm	35%

STUDIES IN CYCLOADDITION

A common reaction to form rings is the Diels-Alder reaction, in which a diene such as 2,3-dimethyl-1,3-butadiene **(1)** reacts with a dienophile, such as β-nitrostyrene **(2)**. Depending on the reaction conditions, this can be a 2+2 cycloaddition, to form two possible isomers of a four-membered ring **(3)**, **(4)**, or a 4+2 cycloaddition to give a 6-membered ring **(5)**. The Woodward-Hoffman rules on the conservation of orbital symmetry predict that the 4+2 reaction will go thermally, whereas a photochemical excitation will produce the 2+2 product. These rules also predict the stereochemistry of the products.



1



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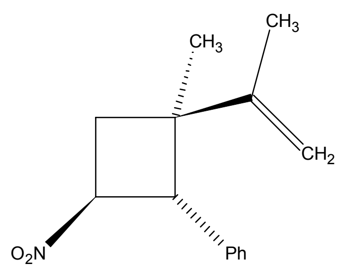

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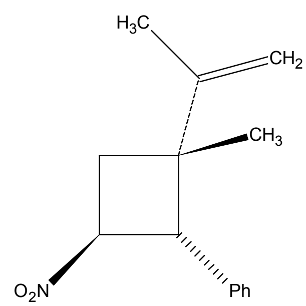

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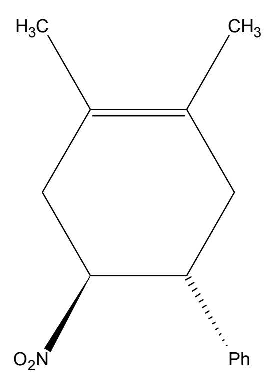
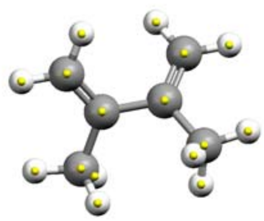
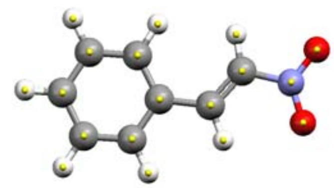


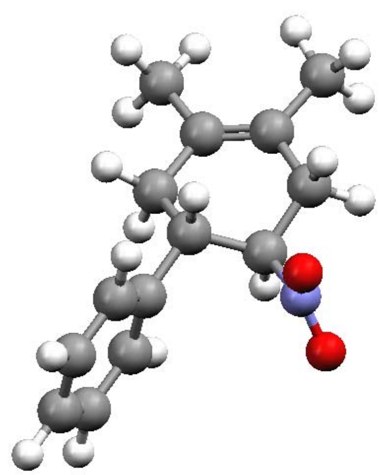
5

In more realistic pictures, the reagents look like this.



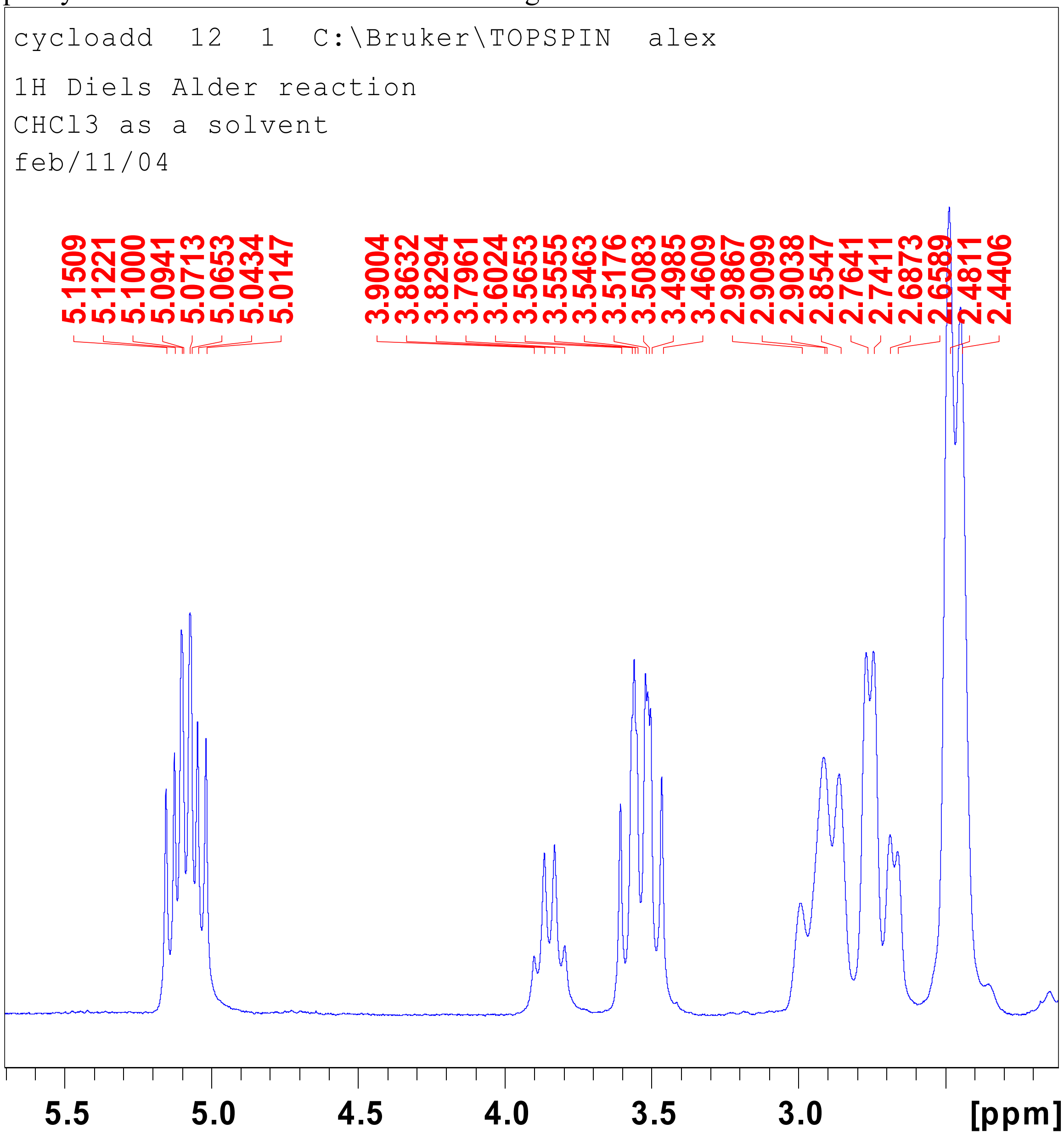


One of the questions about these reactions concerns the stereochemistry – what is the three-dimensional arrangement of the atoms and how can we measure this experimentally? Below is a diagram of the 4+2 product, structure (**5**).

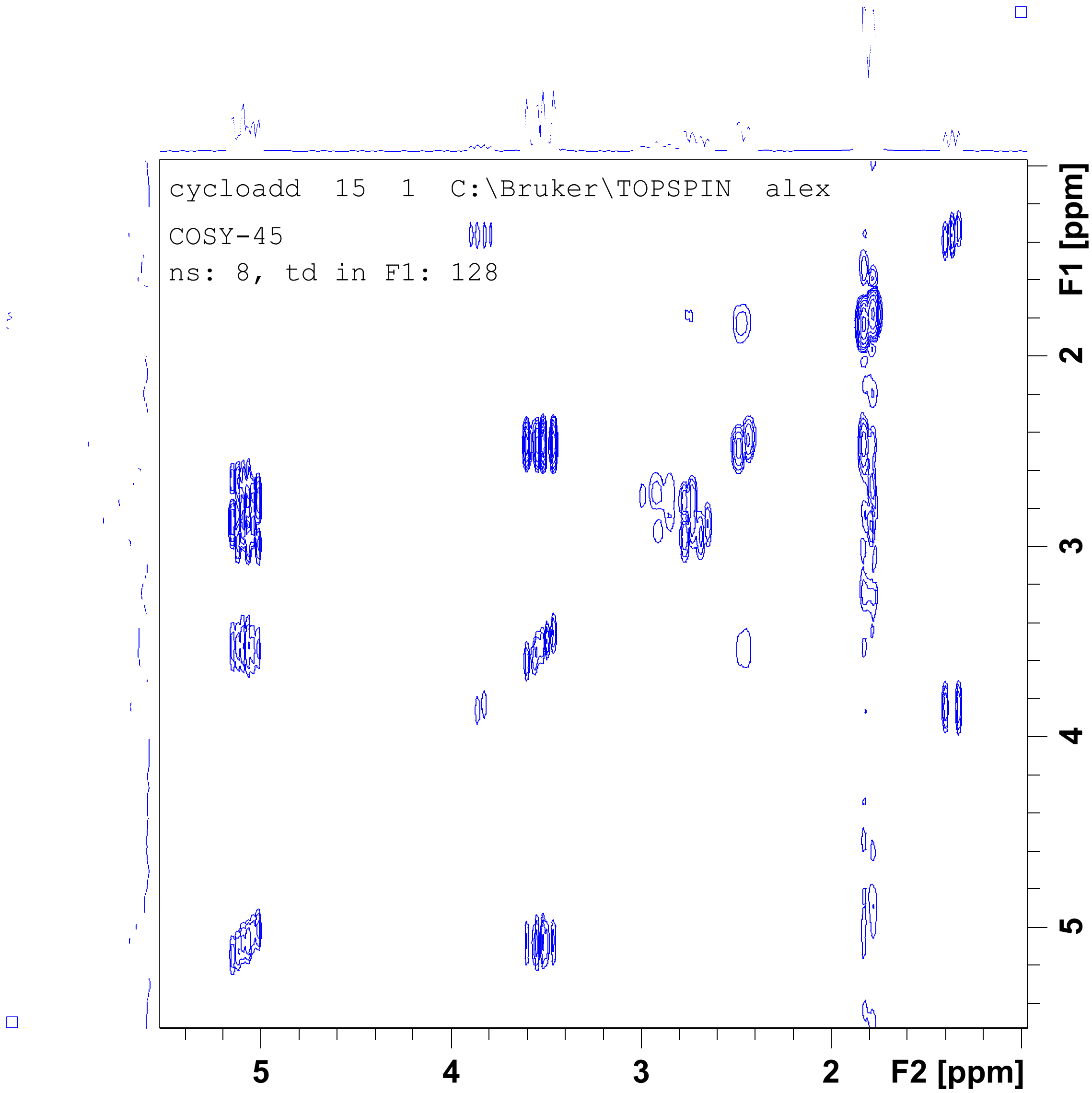


The structure of his molecule can be studied a number of ways. The above diagrams were generated from structures calculated by quantum-mechanical molecular orbital calculations. The experiment yielded good enough crystals for us to do a single-crystal X-ray structure determination.

NMR provides an excellent way of determining the stereochemistry – the splittings of the peaks at 3.5 ppm and 5.1 ppm are very characteristic of the geometry near the nitro and phenyl substituents on the six-membered ring.



This is a classic application of NMR spectral interpretation, but undergraduate laboratories now have access to modern research methods such as 2D NMR. The COSY spectrum of this molecule confirms and broadens our interpretations of the 1D spectrum above.



This spectrum allows us to determine which proton is coupled to which other proton in an exact way.

Summary

Chemistry 3LI3 is a course in which the students get to apply their knowledge from previous courses to a set of new problems. Like the challenges that chemists face, the course applies background from all of chemistry to think through some more ambitious projects and prepares students for further research.