

The Modeling of a Diels-Alder Reaction Mechanism and Expansion into Practical Applications

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1 Abstract

For my project, I would like to combine the programming and modeling I've learned in class and on my own with the organic chemistry background I have. Specifically, I am going to model a simple organic chemistry reaction using VPython and then expand its implications into real world cases of problems and solutions. Because a large complicated molecule and reaction is out of my skill level and ability, I will stick to a simpler reaction and explain why the mechanism and reaction affect our everyday lives.

Using VPython, I will be able to model the stereochemistry of molecules and geometry of the mechanism of the reaction. The reaction I will

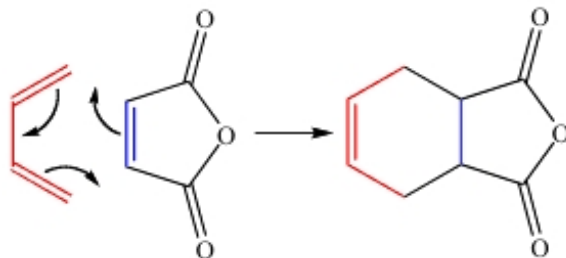


Figure 1: Example of the Diels-Alder reaction between 1,3-butene and maleic anhydride.

be modeling is a Diels-Alder reaction, which is used to create synthetic Eucalyptus Oil and other synthetic materials.

2 Progress

I have already started writing the introduction I will give before presenting my project. It will include a brief background of organic chemistry, the stereochemistry of reactions in general, and an explanation of the particular mechanism I will be modeling. This mechanism, known as a Diels-Alder Reaction, is important in everyday life, because it is a highly efficient method to form stereoselective carbon-carbon bonds in which a conjugated diene reacts with a dienophile (in this case, 1,3-butadiene with maleic anhydride). The reaction is considered to have 100% atom economy, which is increasingly becoming more desirable to dramatically reduce waste in reactions on a large industrial scale. Diels-Alder reactions are also commonly utilized in pharmaceutical research to isolate components of drugs.

I have also started to work on the modeling and programming portion of my project. After installing VPython on my computer, I have looked at several manuals and YouTube videos to help me understand how to operate the program and how I will use it to accomplish my modeling. In addition, I have explored several examples in VPython and manipulated the equations and boundaries to see how the graphics change as a result. In particular, I have looked at two examples of a bouncing ball: one bouncing on a flat surface and once bouncing around and off the walls of a box. Using these and other research, I have found that in order for my molecules to collide, I will use an imaginary "bubble" boundary around each and then calculate whether the boundaries overlap.