

Benchtop NMR for Educational Experiments

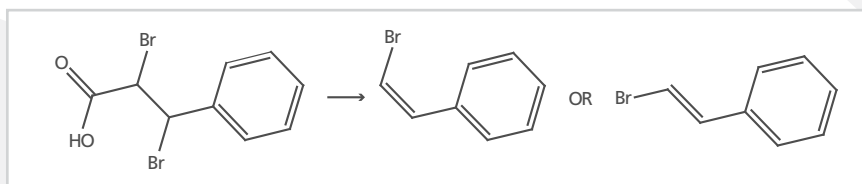
Elimination Reaction

This experiment is designed to teach the practical aspects and principles of the elimination reaction:

Isolation of organic compounds, effect of reaction conditions.

Total experiment time: 1.5 hours in aqueous, 2 hours in acetone

The elimination reaction involves the reaction of a halogenalkane in the presence of heat and a base to produce an alkene. An example is the elimination reaction of 2,3-dibromo-3-phenylpropanoic acid to form 1-bromo-2-phenylethene that takes place via an E1 or E2 reaction depending on the reaction conditions. The reaction is performed in the presence of potassium carbonate:



X-Pulse, a 60MHz benchtop NMR spectrometer can be used to measure the spectra of the starting material and reaction product confirming that the reaction has completed and no starting materials remain. The spectra of the starting material 2,3-dibromo-3-phenylpropanoic acid, along with the final product 1-bromo-2-phenylethene are shown in Figure 1.

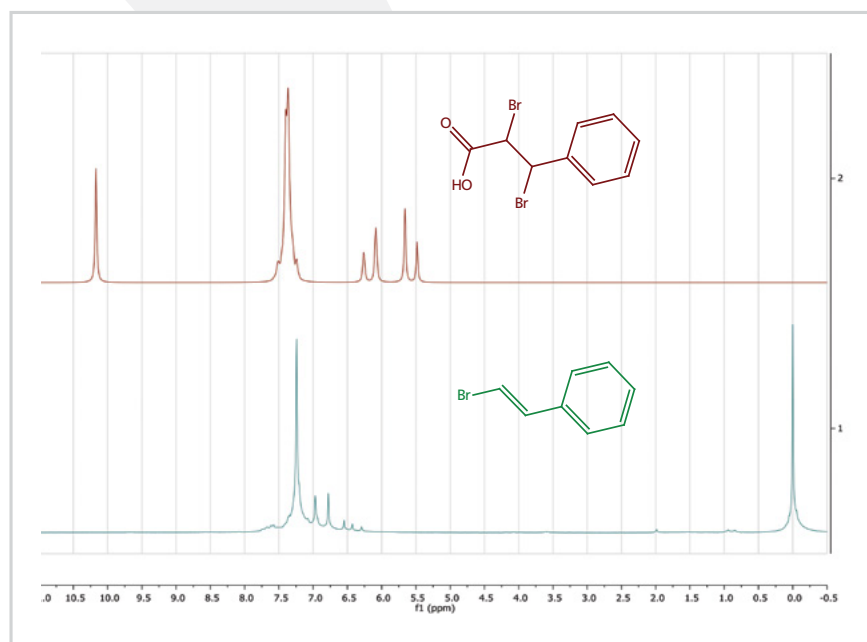


Figure 1. From top to bottom: 2,3-dibromo-3-phenylpropanoic acid, 1-bromo-2-phenylethene spectra

It is clear from these spectra that there is no starting material present in the spectrum of 1-bromo-2-phenylethene. The 1-bromo-2-phenylethene has tetramethylsilane (TMS) added as a chemical shift reference material showing a peak at 0ppm chemical shift.

The product formed can be either a cis- or trans- form of the compound dependent on the solvent chosen for the reaction. In acetone the yield is almost 98% cis form. Whereas in water the yield is 20% cis and 80% trans form of the compound. The peaks due to the different forms (trans peaks are highlighted in blue, cis peaks in pink) are shown in Figure 2.

X-Pulse is a cryogen-free benchtop NMR spectrometer that can easily be sited in the Undergraduate Chemistry laboratory allowing hands-on NMR for students.

A simple to use software interface and standard sampling using 5mm NMR tubes enables a high throughput of samples in a busy laboratory.

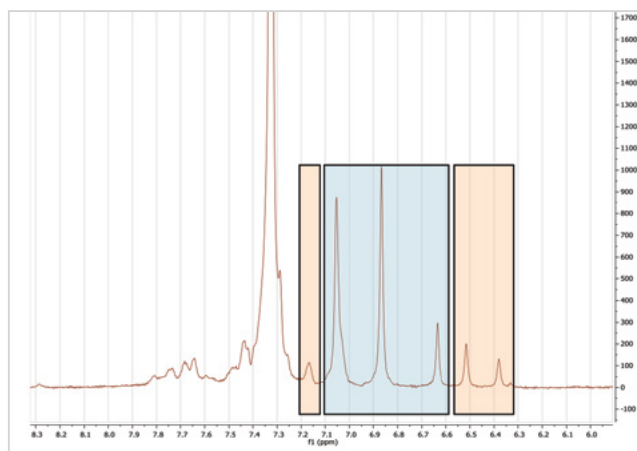


Figure 2. Peaks in the spectrum of the reaction product due to cis (pink) and trans (blue) forms of the compound.

Contact us now for more information
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