Benchtop NMR for Educational Experiments

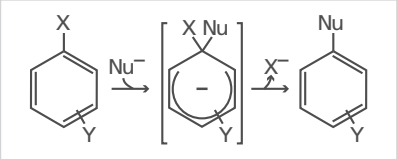
Nucleophilic Aromatic Substitution Reaction

This experiment is designed to teach the practical aspects and principles of the Nucleophilic Aromatic Substitution reaction:

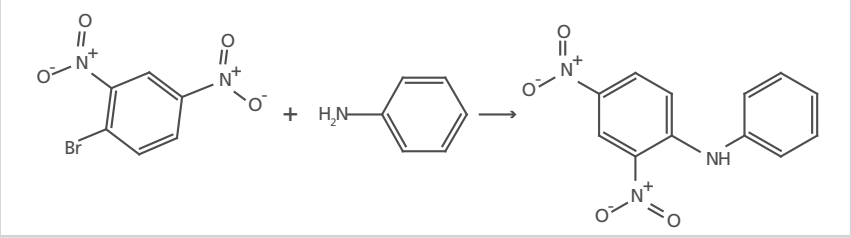
Refluxing, recrystallisation.

Total experiment time: 2 hours

A nucleophilic aromatic substitution is a reaction in which a nucleophile displaces a good leaving group, such as a halide, on an aromatic ring, and is of the general equation:



An example is the reaction is between 1-bromo-2,4-dinitrobenzene and aniline to form 2,4-dinitrodiphenylamine:



X–Pulse, a 60MHz benchtop NMR spectometer can be used to measure the spectra of the starting materials and reaction product confirming that the reaction has completed and no starting materials remain. High quality spectra can be collected within 2 minutes. The spectra of the starting materials 1-bromo-2,4-dinitrobenzene and aniline, along with the final product 2,4-dinitrodiphenylamine are shown in Figure 1 (see over page).

It is clear from these spectra that 1-bromo-2,4-dinitrobenzene and aniline are not present in the spectrum of the product. The 2,4-dinitrodiphenylamine sample has tetramethylsilane (TMS) added as a chemical shift reference material showing a peak at 0ppm chemical shift.

The student can assign the peaks in the spectrum and generate peak integrals in order to verify the identity of the reaction product.

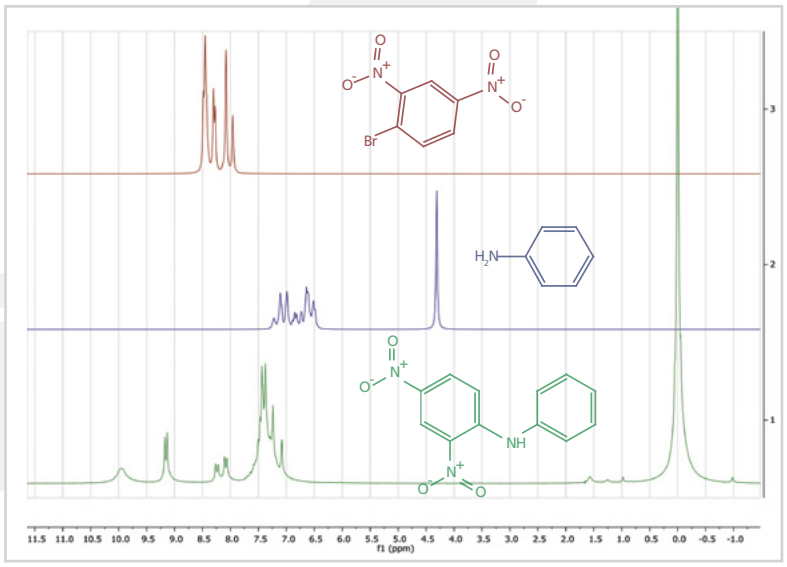


Figure 1. *From top to bottom: 1-bromo-2,4-dinitrobenzene, aniline and 2,4-dinitrodiphenylamine spectra*

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