

Abstract

Nuclear magnetic resonance referred to as NMR is a type of spectroscopy technique used in the organic laboratory to determine the structure of a molecule. Its wide variety of application is essential in the synthesis and analysis of drugs. There are various types of NMR that focus on the chemical distinct environments of a specific elements most used in our lab is H-NMR or proton NMR. In this experiment we analyzed the structure of an unknown compound given its IR and H-NMR and identified the compound as 1,3-dimethyl-5-nitrobenzene. Additionally, we determined the percent composition by analysis of H-NMR of hexane and toluene to be the most accurate in fractional distillation with beads yielding nearly 100% no detection of hexane present in sample. We also identified the mole composition of 4-chlorobenzoic acid and 4-bromoaniline to be in extraction methods. Finally, H-NMR was used in the reduction of 4-Nitro benzaldehyde to 4-Nitrobenzyl alcohol to establish the identity of the product by mole composition.

Introduction

H-NMR is an essential tool for identifying compounds and assessing the purity of a sample. The theory of NMR relies on the spin of nuclei in the presence of a magnetic field to give rise to specific signals unique to a molecule. However, not all atoms are capable of being detected by NMR, this technique may only work with unpaired electrons such as Hydrogen and the isotope of C^{13} . When nuclear spins are not in the presence of a strong magnetic field, they are in a disorder state however when subject to this change in environment they are able to organize themselves in 2 possible spin states aligned with the magnetic field $+1/2$ (lower in energy) or against $-1/2$. The energy difference between the two states is proportional to the strength of the magnet. When a proton exposed to electromagnetic radiation experiences a frequency that is at the same frequency then resonance occurs. At this state the proton that was at $+1/2$ will undergo a momentary change to $-1/2$ spin state (higher energy) absorbing radiation. The energy differences between the states (EM) gives rise to a signal. Each signal corresponds to a chemically unique environment which can then be used to identify the structure of the molecule.

Analysis of H-NMR considers multiple factors such as the location of the signal (up field or downfield) used to identify the presence of electronegative atoms or the presence of multiple bonds. Additionally, the integration of the signal corresponds to the number of hydrogens present in that signal; splitting patterns provide additional information to the connectivity. In some cases, it is helpful to reference additional methods of spectroscopy such as IR which focuses on mainly on the functional groups present in the molecule.

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