**Introduction**

4-allylanisole, or estragole, is a naturally occurring organic compound that is found in various herbs. It is commercially used as a food additive for flavor and in the preparation of perfume fragrances. It is a phenylpropene compound that is composed of a para-disubstituted benzene ring with methoxy and propenyl functional groups, seen as in figure 1. The molecular formula for 4-allylanisole is C_{10}H_{12}O. It has a molecular weight of 148.2 g·mol^{-1} and boiling point of 216°C. The IUPAC designation for this molecule is 1-allyl-4-methoxybenzene. The sample was prepared in deuterated chloroform with 1% TMS.

**1H NMR 1D Spectrum**

The 1D 1H NMR of 4-allylanisole is shown in figure 2. The spectrum was recorded at 800 MHz (1H) with a spectral width of 9842.52 Hz and 16384 complex points. Peaks A and B are downfield resonances centered around 7.07 and 8.11 ppm, respectively. These peaks correspond to the four aromatic protons. Due to the internal symmetry of the molecule H5 and H3 are chemically equivalent and will have identical chemical shifts. Similarly, H6 and H2 will be equivalent. Resolution of the H6/H2 and H5/H3 assignments will be made using the gCOSY spectrum. Peak F is a singlet positioned at 3.72 ppm. This peak will correspond to the methyl protons of carbon 10. This resonance is shifted downfield by the inductive effects of the oxygen atom and will not experience any splitting because of its isolation from other protons. There are two methylene carbons in this molecule, C7 and C9. The two protons of C7 are expected to be further upfield than the protons of C9 due to the pi bond between C9 and C8 (sp2 hybridization). Peak G is an upfield doublet located at 3.30 ppm. This peak must correspond to the two methylene protons of C7 because of its upfield location and the doublet fine structure, caused by the single proton on C8. Therefore, Peaks D and E must be the remaining methylene protons on C9. Two peaks are present around 5.03 and 5.02 ppm because the protons of C9 are chemically inequivalent. The remaining resonance, peak G, must correspond to the methine proton on C8. The fine structure shows a complex multiplet, as expected for H8 due to the four nearby inequivalent protons. Therefore, peak C, at 5.93 ppm, is H8.

**13C NMR Spectrum**

Figure 3 shows the results of the 1D 13C NMR experiment. The spectrum was recorded at 500 MHz (1H) with a spectral width of 31250 Hz and 32768 complex points. Peak A, which is the farthest downfield, corresponds to the quaternary carbon at position 4. This assignment is intuitive based on the aromatic nature of C4 and the proximity to the methoxy group, e.g., compared to the other quaternary carbon at position 1. Peaks G and H are the furthest upfield. Similar to the proton assignments, these peaks correspond to the methyl carbon at position 10 and the methylene at position 7. Peak G is C10, which is shifted downfield due to the inductive effect of oxygen. Therefore peak H is C7. The remaining peaks, B through F, will be assigned using the 13C DEPT and gHMQC data.

**13C DEPT Spectra**

Figure 5 shows the sub-spectrum series of a 13C DEPT experiment. These spectra were recorded at 500 MHz (1H) with a spectral width of 31250 Hz and 32768 complex points. The DEPT experiment shows the hybridization states of the 13C nuclei in 4-allylanisole. The previous assignments for C10 and C7 are

**References and Acknowledgments**

