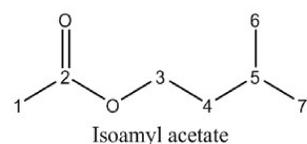


Rhyan Moffitt and Peter F. Flynn

Figure 1



Isoamyl Acetate, also known as Isopentyl Acetate, or banana oil, is an organic molecule with seven carbons. The molecular formula for this molecule is $\text{C}_7\text{H}_{14}\text{O}_2$. There are two

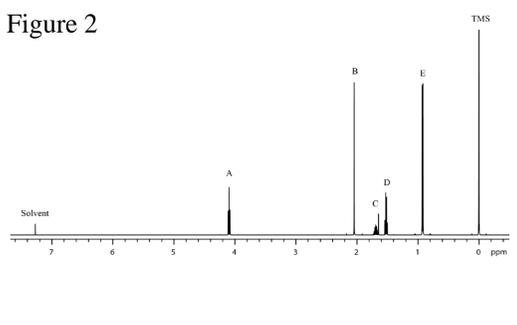
methyl groups branching off of the 5th carbon, which represents the isoamyl (also isopentyl) moiety. The structure of Isoamyl Acetate is shown in Figure 1. This compound is the ester that is formed when combining Isoamyl Alcohol and Acetic Acid.

^1H 1D NMR Spectrum

The ^1H spectrum of Isoamyl Acetate, shown in figure 2, was recorded at 500 MHz. It was recorded using 2048 complex points with a spectral width of 4084.97 Hz (8.16994 ppm.) The resonances of interest lie between 0.5 ppm and 4.5 ppm. All resonances can be assigned by inspection.

The resonance at 7.27 ppm is due to the residual CHCl_3 present in CDCl_3 . The resonance at 0 ppm belongs to the tetramethyl silane (TMS) used for signal referencing. Resonance HA appears at 4.10 ppm, and is assigned to position 3 due in the molecule to its proximity to the electronegative O. HA is a triplet, which is consistent with assignment of the resonance to position 1 as it is one of two positions in the molecule with adjacent methylene groups. Resonance HB at 2.05 ppm is a singlet, and is assigned to position 1 in molecule since that nucleus is the only one in the molecule that is predicted to have no coupling to other protons. Resonance HC is a septet that is assigned to position 5 in the molecule, which has two adjacent methyl groups attached to it.

Figure 2



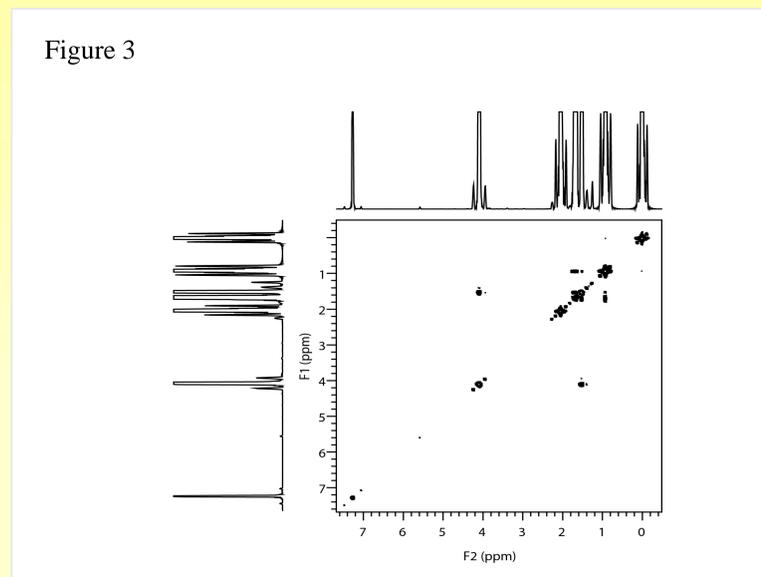
Peak	Chemical Shift (ppm)
A	4.10
B	2.05
C	1.69
D	1.53
E	.930

Resonance HD, at 1.53 ppm is a pseudo-quartet meaning there are three neighboring hydrogens confirming that resonance HD is 4 and is actually a doublet-of-triplets. This fine structure arises due to the interaction of the methylene group present at position 4 in the molecule with the adjacent methylene group at position 3 and the methine proton at position 5. The magnitude of the coupling between the methylene protons at position 4 and the methine proton at position 5 is such that the triplet fine structures overlap to produce the apparent quartet. The last resonance, HE, at 0.930 ppm can be assigned to both of the methyl groups and positions 6 and 7 in the molecule due to the low chemical shift value and because the resonances appear as a doublet due to the coupling from the adjacent methine proton at position 5.

gCOSY 2D NMR Spectrum

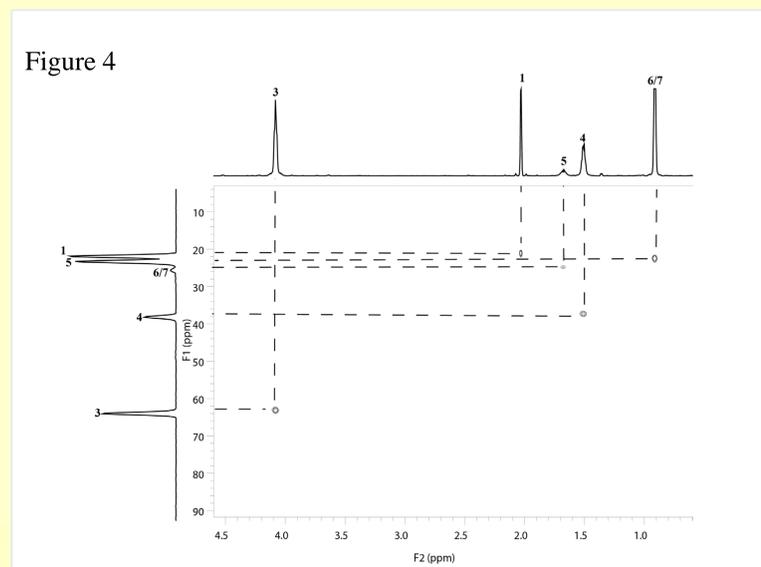
The information from the gCOSY confirms the assignments made using the ^1H NMR spectrum.

Figure 3



HMQC 2D NMR Spectrum

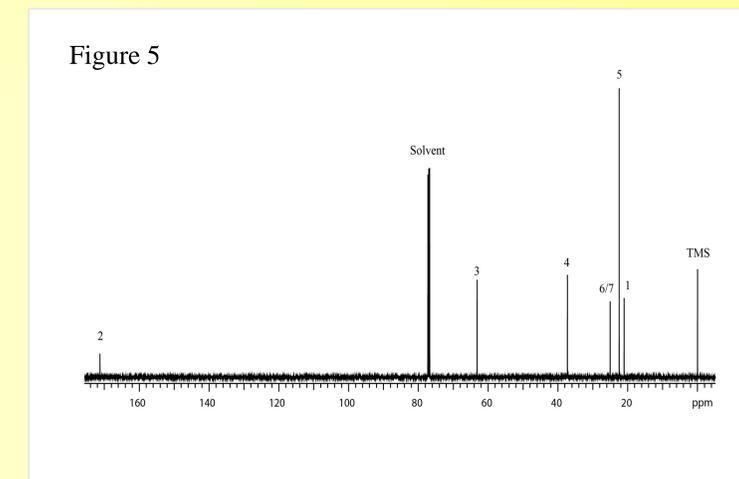
Figure 4



^{13}C 1D NMR Spectrum

The ^{13}C spectrum of isoamyl acetate is shown in figure 5. The data was recorded at 500 Hz using a spectral width of 22727.3 Hz (45.4546). Through process of elimination the last resonance at 171.257 ppm can be assigned to position 2 that has no hydrogens bound to it.

Figure 5



Peak	Chemical Shift (ppm)
1	21.053
2	171.257
3	63.165
4	37.308
5	22.465
6/7	25.052

Results

The ^1H resonances present in the spectrum were assigned by inspecting the chemical shifts and fine structure of each resonance. These assignments were then used in the 2D HMQC spectrum to assign the ^{13}C resonances. Note that the carbonyl ^{13}C resonance was unambiguously assigned by simple elimination.

References

Claridge, Timothy D. W. *High-Resolution NMR Techniques in Organic Chemistry*. Amsterdam: Elsevier, 2009.
Keeler, James. *Understanding NMR Spectroscopy*. Chichester: John Wiley & Sons, Ltd, 2010

The 2D Gradient-Enhanced Heteronuclear Multiple Quantum Correlation spectrum is an experiment that shows the chemical shift correlations of carbons and hydrogens directly bound to one another. This experiment was recorded at 800 MHz with spectral widths of 7575.76 Hz (9.4697 ppm) in the direct (^1H) dimension (F2, horizontal axis) and 42238.6 Hz (52.79825 ppm) in the indirect (^{13}C) dimension (F1, vertical axis). The direct dimension was recorded with 2272 complex points in the direct, t2, dimension, and 450 complex t1 points in the indirect dimension. Using the projections of the 2D resonances to the carbon dimension allowed the ^{13}C resonances to be assigned directly through their correspondence with the already assigned hydrogen resonances.