Acquisition Time and Spectral Width in NMR
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When performing NMR experiments, it seems counterintuitive that a short acquisition time is required for a larger spectral width. The nature of this effect stems from the fact that FID data is acquired in the time domain, and then Fourier transformed into the frequency domain to yield the familiar NMR spectrum. Let's look at this process in more detail with the goal of achieving both a quantitative reason for the result, as well as a qualitative understanding of the relationship between data acquisition time (time domain) and spectral width in the resultant NMR spectrum (frequency domain).

Quantitative Understanding

For a sine wave to be adequately digitized as it decays in time (such as a FID in NMR), the number of points used in the acquisition has to equal twice the total number of cycles observed. Let $NP =$ Number of Points, then,

$$NP = 2 \ (\# \, \text{Cycles})$$

This is based on a rule of digitalization called the Nyquist Principle. Following this principle prevents any artifacts in the data once it is Fourier transformed into the frequency domain. We can also divide each side of the equation by seconds and write:

$$\frac{NP}{\text{sec}} = 2 \left(\frac{\# \, \text{Cycles}}{\text{sec}} \right)$$

In NMR, the Dwell Time, DW is defined as the number of seconds between points during data acquisition in the FID, which is the same as seconds/point such that

$$DW = \frac{\text{sec}}{NP}$$

Consequently, $1/DW$ is the number of points per second, or

$$\frac{1}{DW} = \frac{NP}{\text{sec}} = 2 \left(\frac{\# \, \text{Cycles}}{\text{sec}} \right)$$

The total number of cycles per sec is the same as the total window of observed Hz, and is called the spectral width, SW. As a result of the definitions so far,

$$\frac{1}{DW} = \frac{NP}{\text{sec}} = 2 \bullet SW$$

Another couple of definitions come into play when digitizing a FID in NMR. The Acquisition Time, AT is simply the total time interval of acquired data in the time domain. With a little additional thought, we realize by definition that the if we multiply the seconds per point by the total points, we get AT and so,

$$AT = \left(\frac{\text{sec}}{NP}\right) NP$$

And by substitution,

$$AT = \left(\frac{\text{sec}}{NP}\right) NP = DW \bullet NP$$

Then, by further substitution of *DW*,

$$AT = \frac{NP}{2 \bullet SW}$$

Now we see clearly, based on definitions and the rule of digitalization, that if the spectral width in the spectrum, *SW*, is increased, the acquisition time in the FID, *AT,* decreases for a fixed *NP*. This expression is so basic to the way FT-NMR works, it is sometimes referred to as the "fundamental equation of NMR data acquisition". It links the time domain (on the left) to the frequency domain (on the right). Most explanations of this point start by merely stating the equation, but don't actually explain why it is used, and how it originates.

On a Varian spectrometer, *DW* is not a parameter made available to the user, but the fundamental equation of data acquisition is barely comprehendible without a definition and discussion of *DW*. Instead, on a Varian, *DW* is hidden, and if the user changes *SW*, *AT* is held fixed, and the spectrometer automatically re-computes the appropriate *NP* to maintain the equation. This is completely baffling unless the user knows what's going on: the spectrometer software is actually doing the user a favor by maintaining a required equality.

This is an appropriate time to point out that the digital resolution, *R*, in the frequency domain is defined as:

$$R = \frac{1}{AT} = \frac{2 \bullet SW}{NP}$$

which yields *R* in units of sec^{-1} or Hz/point, which is logical for NMR data in the frequency domain.

Qualitative Understanding

A qualitative appreciation of the fundamental equation of NMR data acquisition is gained by keeping in mind that FID data is collected in the time domain (typically seconds), and then Fourier transformed into the frequency domain (reciprocal time, typically sec^{-1}, or Hz). The reciprocal relationship between the data acquired and the data produced helps to understand more readily why a large spectral width, or *SW*, uses a short acquisition time, *AT*.

Note

It is incorrect and confusing to refer to *SW* as the "sweep width". That term is a carryover from the days NMR data sets were acquired in a continuous wave mode where the magnetic field strength was swept over time. Today, the magnetic field is held constant, the sample is pulsed, FID data acquired, and Fourier transformed to yield an NMR spectrum in the frequency domain. The modern approach provides data of higher quality.