Apodization.

This is a short handout to introduce apodization and digital resolution. All of the functions discussed are available on GE/Nicolet NMR spectrometers. The sample used was 0.032 M menthol/CDC13, and the proton spectra were acquired using the GN500.

Apodization is an umbrella term that is used to imply a manipulation of the FID to either increase signal-to-noise (S/N) or resolution. You usually can gain either S/N or resolution, but not both. These two aspects of apodization will be discussed below.

Digital Resolution

Digital resolution is defined: Rd = 1/AT = 2(SW)/NP

where Rd = digital resolution
AT = acquisition time
SW = total spectral width
NP = total # of data points (block size)

The digital resolution is the interval between data points in the frequency spectrum. If you have inadequate digital resolution, you can totally mask spectral features. Figure 1 shows an example of this problem. An easy and quick way to determine the correct choice of NP to insure adequate digital resolution is illustrated in figure 2. The FID decays with a time constant Ae-a2. You need to choose the NP so that the FID decays to zero by half-way through the FID. The minimum NP to assure adequate digital resolution in figure 2 is 32K. Choosing NP in this manner should also insure that you have enough infornnation in your FID to adequately characterize all lines in the spectrum. For example, in figure 1, no matter what resolution enhancement technique one uses, the lower spectrum will never match the resolution of the upper spectrum because the data collection (i.e., the FID) does not contain enough information. This would be comparable to collecting 4K data points in figure 2 and then zero-filling (ZF) to 32K. The FID must decay to zero by the end of the FID to fully characterize all frequencies.

Zero-filling is a method of adding data points to an FID if insufficient digitization is present to adequately characterize all lines in the spectrum. It is a resolution enhancement technique, and is illustrated in figure 3.

Signal-to-Noise (S/N) Enhancement

Line broadening, whether Lorentzian or Gaussian, improves S/N but causes a broadening of lines - hence the name. The optimal line broadening to use is the linewidth at half-height (LW1l2), which produces the so-called "matched-filter" apodization. If you have a spectrum with a flat baseline, there is no need to use line broadening. It is only useful when a spectrum contains too much noise for your purposes. An example is shown inf figure 4. Another example is shown in figure 5, where the end result of too much line broadening is illustrated. The shapes of the Lorentzian and Gaussian line broadening functions are shown in figure 6. Lorentzian line broadening is chosen with EM, whereas Gaussian line broadening is chosen with GM. In both cases the extent of line broadening is set with LB.

Resolution Enhancement

Two common methods of resolution enhancement are the double apodization (DM) and sine bell (MS) apodizations. If either DM or MS is used on a GE/Nicolet instrument, you will be prompted for an additional parameter. The DM parameter is a combination of variables, while the MS parameter specifies a phase shift (to the left, measured in degrees). These functions are shown in figure 7, while figure 8 shows the result of applying these functions to an FID. Resolution enhancement functions modify the appearance of an FID to increase signal in the appropriate area as indicated in figure 7. You should choose the combination of functions that best fit your FID and allow maximum enhancement without distortion of the resultant spectrum. Resolution enhancement usually results in an increase in noise in a spectrum, so optimal results are obtained with a spectrum with a good S/N.