NMR NOTES #6

Using S and SS pulses on Unity and UnityPlus

The S and SS shaped pulses, created for the waveform generator on the Unity consoles, provide a convenient mechanism for observing a proton spectrum without exciting the water solvent resonance. The shaped pulse provides suppression at the carrier frequency, which should be positioned on top of the solvent signal, and excitation maxima at frequencies symmetrically placed above and below the carrier frequency. The actual frequency of the maxima is controlled by the pulse width, and is specified when the pulse is created. The command `makeSS(1500)` was used to create the standard SS pulse file named SS7342g.RF, which requires that the pulse width be 734.2 uSec and provided excitation maxima at +/- 1500 Hz from the carrier. Likewise, the shape file S4452g.RF is an S pulse with maxima at +/- 1500 Hz and requiring a pulse width of 445.2 uSec. In order to use either pulse, it is necessary to reduce the transmitter power significantly since the pulses are quite long. Start with a pulse width/pulse power combination at relatively low power: 26.2 uSec pw90 at tpwr=45 for instance. Either measure this value directly or get a 'good' value from the pw90 table. Now calculate the power level required for 90 degree pulse of the appropriate pulse width (734.2 uSec). 734.2/26.2 gives a pulse width factor of 28.02. The pulse width modification table shows a value of 28.1 at -29 db, so we will use this. The transmitter power is then 45-29=16. Add 6 db to this value and use this for the transmitter power level (tpwr=16+6=22). The extra 6 db accounts for the fact that we are supplying power to two lobes, above and below the carrier position. The SS pulse will give all positive peaks and a relatively broad null region at the carrier position. The S pulse will give a 180 degree phase shift at the carrier, a sharper null at the carrier, and a broader pass band on either side. In addition, the S pulse will be shorter than the SS pulse for the same excitation maxima, resulting in less frequency dependant phase shift correction.

The long shaped pulse results in the time domain signal effectively beginning in the middle of the pulse, before data acquisition can begin. This leads to a large, negative left phase correction and a concomitant baseline roll. In order to eliminate the large phase shift and baseline roll, the data set is shifted right several data points, and the missing points are back calculated using the linear prediction software. Each data point added with increase the left phase correction by 360 degrees. Left shift and linear predict a sufficient number of data points to make the left phase correction positive. The `calfa` command can now be used to calculate a new alfa delay value which will make the left phase correction very close to zero after the next data collection. At this point the spectrum should be properly phased without any appreciable baseline roll. All of these phase shift corrections can be made automatically with the `fixSS` macro on the spectrometer. This macro cannot be applied successively - it corrects the left phase parameter assuming no existing correction, and will not add a correction on top of an existing correction. If you need to make successive approximations to correct the phase, only the first can be done automatically.

The S and SS pulses can be used either as a standard 1D observe experiment, using the sh2pul pulse sequence, as part of a 2D noesy experiment, using the SSnoesy sequence, and as part of a 2D roesy experiment using the Ssroesy sequence. All three macros, sh2pul, SSroesy, and SSnoesy are defined on the system and will automatically set up the necessary parameters. You will only have to calibrate the pulse power value.

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