

## How to Shim on a Varian

The term ‘shimming a magnet’ is a piece of NMR jargon that harks back to the early days of NMR spectroscopy. Originally, permanent magnets were used to provide the external magnetic field. To obtain the most homogenous field across the sample, the pole faces of the magnet had to be perfectly aligned, and to accomplish this, small pieces of wood, or ‘shims’, were hammered into the magnet support, so as to physically move the poles relative to each other. Luckily, nowadays you will not be required to bring hammer and wooden shims to the spectrometer. Shimming is accomplished by changing the applied current for a set of coils surrounding the probe. This applied current will create small magnetic fields in the region of your sample that will either enhance or oppose the static magnetic field. Your goal will be to adjust these coil fields by a series of mouse clicks to obtain the most homogeneous magnetic field across your sample, which is usually observed as an increase in the lock signal.

It is important for you to have a basic understanding of line shape so you can judge when: (1) your shimming is off, and (2) you need to spend more time shimming your sample. The best way to avoid problems is to establish a procedure, such as the one detailed below.

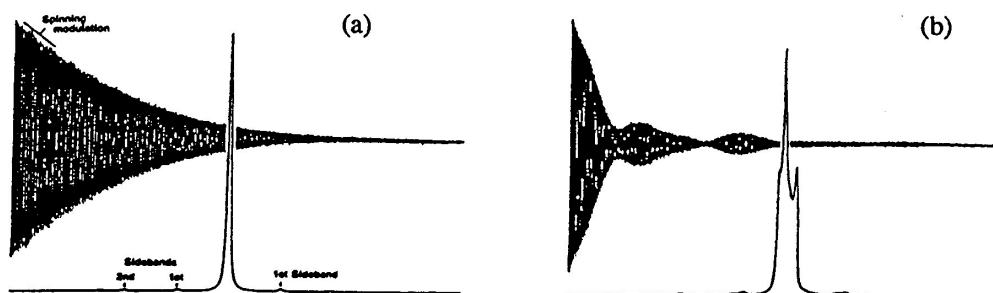
- I. Always load a shim library when you sit down at the instrument. You should never assume the previous user left the instrument with a standard shim library loaded. Without reloading standard shims, you will have to start where the last person stopped - and that might include someone who shimmed for a short sample, a bad tube, a viscous sample, etc.
- II. Be aware of lock parameters, especially if you only shim on the lock display. Establish lock transmitter power and gain levels that work for most of your samples. If you encounter a sample that seems to require an unusually high power or gain setting, there is a problem with your sample and/or the instrument, and shimming on the lock level may be difficult or impossible.
- III. Shimming problems are confirmed only if the problem is visible on every peak in your spectrum. If, for example, only one peak is doubled, the

problem is sample related, and can't be shimmed away. Remember, anomalies close to the base of intense single lines may not be visible on less intense peaks unless the vertical scale is increased.

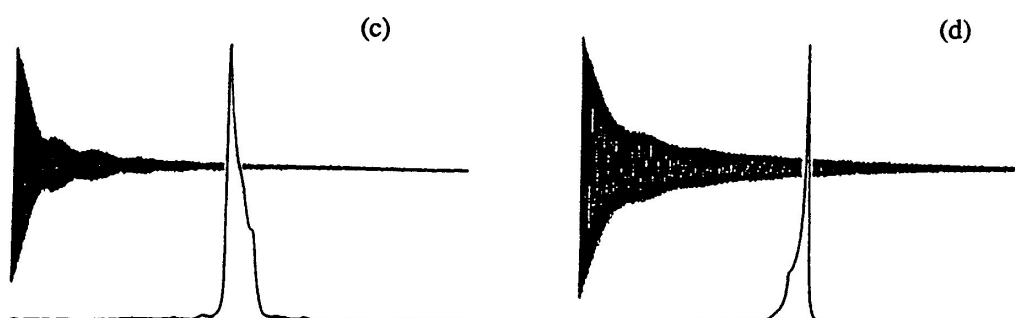
- IV. Establish a shimming method. Shimming is an 'art form' that requires patience and practice. You should always approach shimming with some method that works for you to give acceptable results. Example: load a shim library; adjust the lock level to a maximum with Z1, then Z2, then Z1, then Z3, and then Z1.
- V. Spinning side bands should always be below 2%. If spinning side bands are above 2%, turn off the spinner air, optimize the X and Y shims, then turn the spinner air back on and re-optimize Z1, Z2, and Z3. If this does not solve the problem, consider transferring your sample to another tube.

Knowledge of correct line shape can help you correct problems such as those shown in Figure 1. Although the peak in Figure 1b may have a line width at half-height that is less than 0.50 Hz, it is obviously poorly shimmed. You should never accept a poorly shimmed line shape such as is shown in Figure 1b, where a single line is expected.

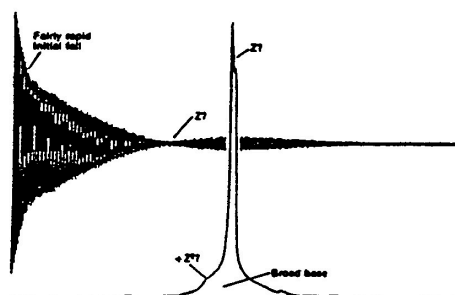
On the pages that follow are some line shape defects and the shims that should be adjusted to correct the problem. You will also notice that the FID will show the problem as well, but may not be as easy to diagnose. In general, odd-order shims (Z1, Z3, Z5) affect the line shape symmetrically while even-order shims (Z2, Z4) cause a non-symmetrical line shape. The higher the order (Z4 is higher order than Z2), the lower (closer to the base of the peaks) the problem is observed.



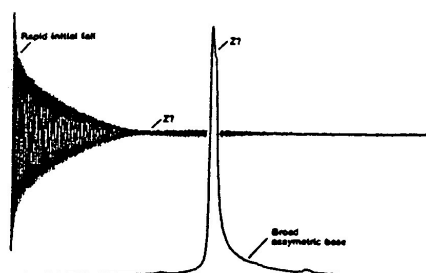
**Z1 --** A "good" FID and a spectrum with small spinning sidebands are shown above in (a), but when the "Z" shim is changed (b), a characteristic beat in the FID is obtained, and the spectral line broadens and manifests structure that is an indicator of Z1 inhomogeneity.



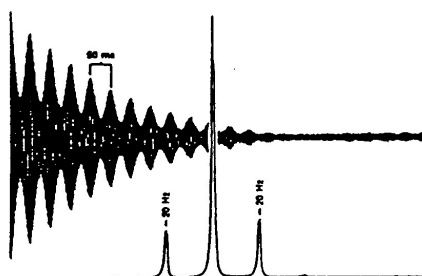
**Z2 --** The asymmetric shape of the above peak (c) is typical of a mis-set Z2 shim. Note that the beats in the FID are less pronounced than in the diagram for Z1 (above, figure b) and that the initial descent is steeper. If the Z2 shim is mis-set in the opposite direction, then the asymmetry is reversed (d).



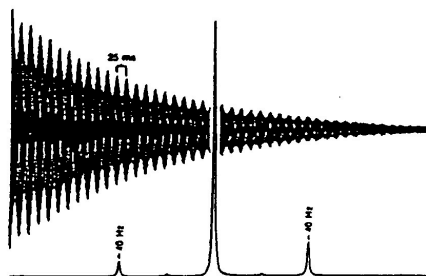
**Z3 --** Although the broadened base of this peak is typical of a mis-set Z3 shim as is the rapid initial descent of the FID, there are also hints of +/-Z1 and +Z2 in the lineshape.



**Z4 --** The very rapid initial fall of the FID and the pronounced asymmetry are typical of a mis-set Z4 shim. Note that in contrast to the effect of the Z3 shim effect in the previous diagram, there is very little evidence of Z1 or Z2, suggesting that the Z3 and Z4 shims windings are staggered slightly; i.e., their origins differ. Reversal of current in the shim naturally reverses the asymmetry.



**X or Y --** The formation of echoes in the FID every 50 ms is clearly visible, and first-order spinning sidebands 20 Hz away from the main spectral line can be seen. First-order spinning sidebands are separated from the main peak by the sample spinning rate (20 Hz).



**XY or X<sup>2</sup>-Y<sup>2</sup> (R<sup>2</sup>) --** Echoes are now formed every 25 ms (see previous diagram), and the spinning sidebands are "second-order," i.e., 40 Hz away from the main line, which is twice the sample spinning rate. The difference in the two sidebands' heights is often seen for mis-set XY or X<sup>2</sup>-Y<sup>2</sup> shims.

**Figure 1.** From G. Chmurny and D. Hoult, "The ancient and honorable art of shimming." *Concepts in Magnetic Resonance*, 1990, 2, 131-149.

With these drawings, you are armed with the knowledge of which shims cause certain artifacts. Be forewarned, however, that the individual shims 'talk' to other shims and changing a given shim will affect another set of shims. Now, for step-by-step procedure:

### Explanation of Types of Commands Found in this Handout:

1. The VNMR software and the UNIX operating system are both case sensitive. This means that the computer distinguishes whether the letters are entered in upper case (*i.e.* CAPITALS) or lower case. The user must be careful to type the correct case for each letter in a command.

*Example: **jexp1** is not the same as **JEXP1***

2. Some commands are line commands and are typed in by the user followed by a return (a Return is assumed for typed **bold** text commands).

*Example: **su***

3. Some commands are executed by clicking a mouse button with its pointer on a "button" found on the screen. The execution of these commands are indicated by a two letter designation (LC {left click}, RC {right click}, or CC {center click}) followed by a word or words in **shadow** that would appear in the button.

*Example: LC **Main Menu***

This means to click the left mouse button with its pointer on the button that says "Main Menu".

4. Some commands are executed by the mouse itself. These commands are indicated by a two letter designation (LC, RC, or CC) and a description of what the user should do in parentheses.

*Example: LC (at 6 ppm)*

This means to click the left mouse button with the mouse cursor positioned at 6ppm.

5. Parameters are entered by typing the parameter name followed by an equal sign, the value, and a return.

*Example: **nt=16***

\* \* \* \* \*

### **Shim on the Sample**

In the VNMR ACQUISITION Window (opened by LC on **acq1**):

LC **SHIM**

connect to interactive shim window.

LC or RC **Z1C** -4+ button

adjust Z1C to maximize the lock level

**NOTE:** Some instruments do not have a Z1C or Z2C. If this is the case, use the Z1 or Z2 -64+ button.

LC or RC <b>Z2C</b> -4+ button	adjust <b>Z2C</b> to maximize the lock level
LC or RC <b>Z1C</b> -1+ button	adjust <b>Z1C</b> to maximize the lock level
LC or RC <b>Z2C</b> -1+ button	adjust <b>Z2C</b> to maximize the lock level
LC or RC <b>Z1</b> -16+ button	adjust <b>Z1</b> to maximize the lock level
LC or RC <b>Z2</b> -64+ button	adjust <b>Z2</b> to maximize the lock level
LC or RC <b>Z1</b> -4+ button	adjust <b>Z1</b> to maximize the lock level

- a. Repeat **Z1C** and **Z2C** shimming *interactively* (*i.e.*, if one is changed, the other should be readjusted) until maximum lock level is achieved. You may want to re-optimize the lock phase now if large changes of these shim gradients have been made.
- b. Then, **Z1** and **Z2** are adjusted *interactively* until maximum lock level is reached (usually starting with -16+, then -4+).
- c. At this point, it is good to close the shimming window and do a quick acquisition to see the lineshape and determine which, if any, shims need adjustment. To do this;
  - i. LC **Close** on the acqi window.
  - ii. Setup the appropriate experiment, if you haven't done so.
  - iii. **nt=1** to set to a single scan.
  - iv. **ga** to acquire and process the data.
  - v. Expand and look at the peaks for the distortions shown in Figure 1.
  - vi. To check  $LW_{1/2}$ , LC **Cursor**, LC on a singlet (preferably  $CDCl_3$ ), **nl dres**.
  - vii. Adjust shims as necessary.
- d. Normally, **Z3** is not changed. If **Z3** is changed, **Z1** and **Z2** will need to be re-optimized. First attempt to optimize using -4+ button. When you get it as good as possible, acquire a spectrum and check lineshape. If it is still unacceptable, try the following;
  - i. In the **Shim** window in **acqi**, note the Lock value.
  - ii. Note **Z3**, then adjust **Z3** in one direction until your lock level drops ~10%.
  - iii. Optimize **Z1** and **Z2** and see whether the new lock value is better than where you started. If it is, continue to change **Z3** in the same direction with optimization of **Z1** and **Z2** until you reach a maximum. If the level was lower in after the first optimization of **Z1** and **Z2**, adjust **Z3** in the opposite direction past the original value (noted in ii.) and optimize **Z1/Z2**. Continue to optimize as necessary.

**NOTE:** *No shimming on **Z4** should be needed for routine experiments, unless you are observing a sample with very different physical properties from those of the standard or a sample of unusually short length.*

When you finish shimming, optimize the lock phase one last time and check that the lock level is between 40 to 90, then

LC **Close**

close Acqi window.