APPENDIX C
OPTIMIZING SHIMMING

Shims are a set of coils inside the magnet that induce changes in the shape of the magnetic field. Each shim produces a specific change in the magnetic field that can be easily shown. Like system lock, you have a choice between automatic and manual shimming.

- For automatic shimming, you can skip this section or read the next two subsections below.
- For manual shimming, follow the procedure described in "Manual Locking" below.

Automatic Versus Manual Shimming

Why would somebody prefer manual shimming over automatic shimming? Experienced users often prefer manual shimming because they can usually optimize shims faster than automatic shimming can. These users then can eliminate the time for automatic shimming from the experiment. On the other hand, manual shimming takes some skill and patients to be effective. Many users prefer to let the system shim automatically.

Automatic Shimming

Automatic shimming is done by default during a standard experiment, refer to "8. Running a Standard Experiment" on page 21. During a custom experiment, automatic locking can be turned off or left on as part of the acquire phase of the experiment, refer to "9. Running a Custom Experiment" on page 22.

Manual Shimming

The next few sections describe the shim interactions and how to adjust the various shims. Understanding the effect of the various shims on symmetry of the resonance is important in simplifying the shimming process. Consider the following two points:

- The effect of a given shim on the spectral lineshape.
- How the shims interact with each other.

Understanding how the shims interact is critical to simplifying the task of shimming. Pure shim gradients produce a very specific and predictable effect on the magnetic field and, to a lesser extent, on the resonance lineshape.

Shim Interactions

The following sections show theoretically predicted changes in lineshape caused by changes in shim DAC values. Shim sets with pure shims, such as the Varian Ultra•nmr shims, follow the theoretically predicted response very closely. Other shim systems, with more interactions between shims, produce somewhat different results.

Theoretically Perfect Lineshape and Effect of Z1 Shim

Figure 5 shows a theoretically perfect lineshape (at left) produced in a perfectly homogeneous field (at right). The magnetic field shape appears as a flat line, indicating that the magnetic field does not change across the length of the sample.

Figure 6 shows how changing the linear shim Z1 affects the lineshape and the magnetic field.

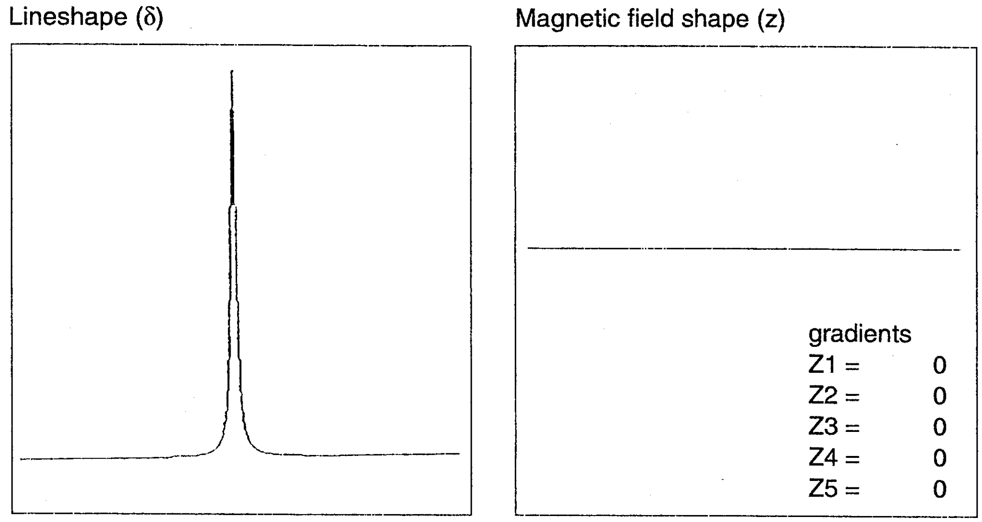

Figure 5. Theoretically perfect lineshape

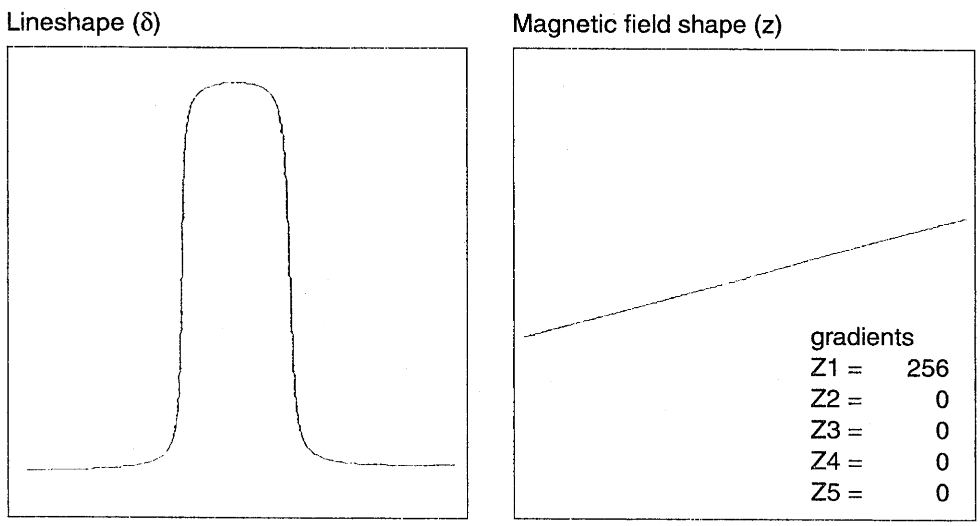

Figure 6. Effects of linear shim Z1

Effects of Even-Order Shims Z2 and Z4

Figure 7 shows the effect of the even-order shims, Z2 and Z4, on the lineshape. Notice that a positive misadjustment of both shims produces an upfield tail on the peak. If Z2 and Z4 are misadjusted in the negative direction, the asymmetry occurs on the downfield side of the peak. The difference between Z2 and Z4 is in the height of the asymmetry. The Z2 shim causes asymmetry higher on the peak than Z4.

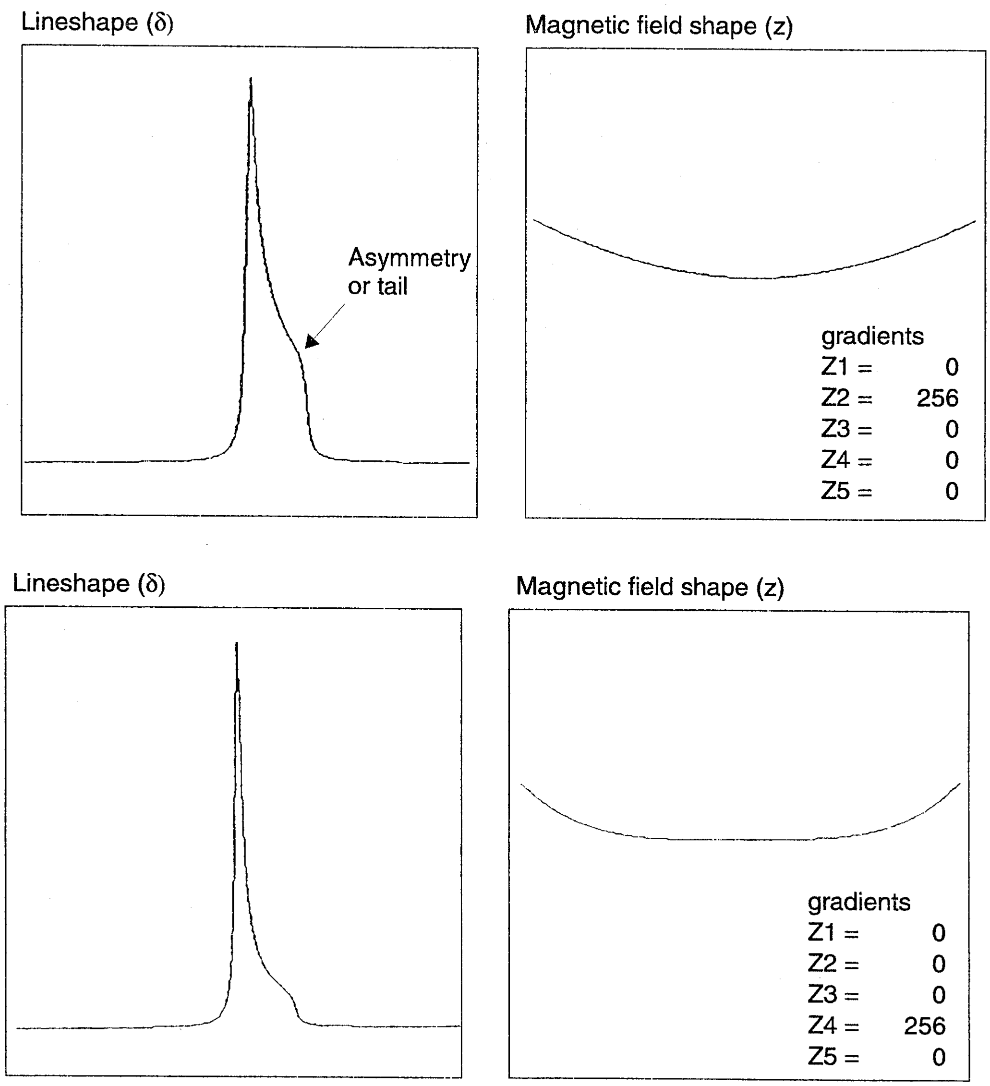

Figure 7. Effects of even order (parabolic) shims Z2 and Z4

Effects of Odd-Order Shims Z3 and Z5

Figure 8 shows the effects of the odd-order shims Z3 and Z5 on the lineshape. The odd-order shims cause broadening of the peak and therefore affect resolution.The Z5 shim is unavailable on systems with 13-channel shim sets (`shimset=1`).

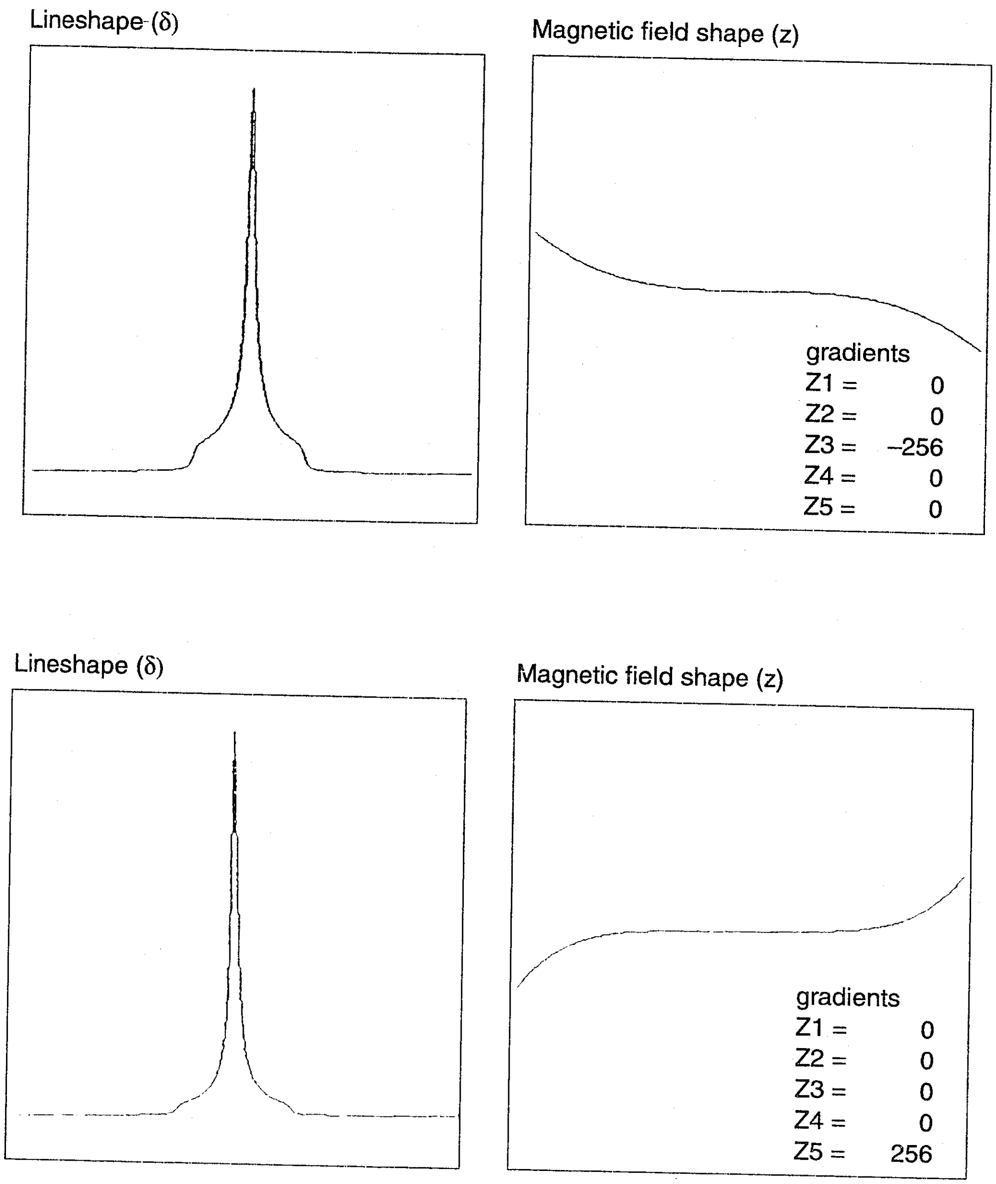

Figure 8. Effect of odd order (non-linear) shims Z3 and Z5

Effects of Misadjusted Shims

Figure 9 shows two examples of the effects when more than one shim is misadjusted. This is the typical case with real samples. The complex lineshapes make simple visual analysis difficult. A procedure for correcting the shims is provided later in this section that can be used as a guide when adjusting shims.

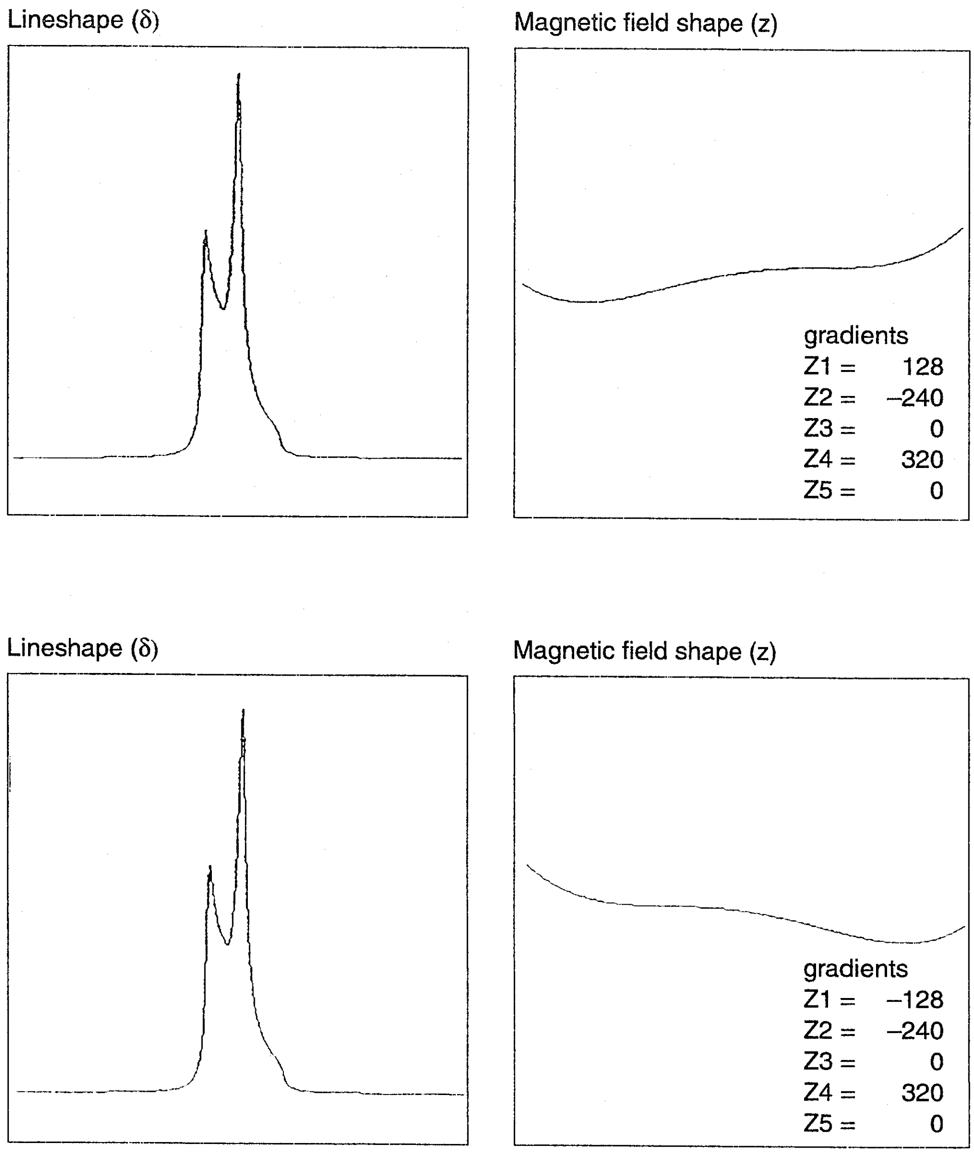

Figure 9. Effects of misadjusted shims

Effects of Non-Spin Shims

Figure 10 shows the effect of the non-spin shims on the spectrum (note that Z3X and Z3Y are not available on 13-channel shim systems). If set wrong, the first-order non-spin shims (X, Y, ZX, and ZY) can cause first-order spinning sidebands. XY and X2–Y2 can cause second-order spinning sidebands. High-order non-spin shims can cause a broad peak base.

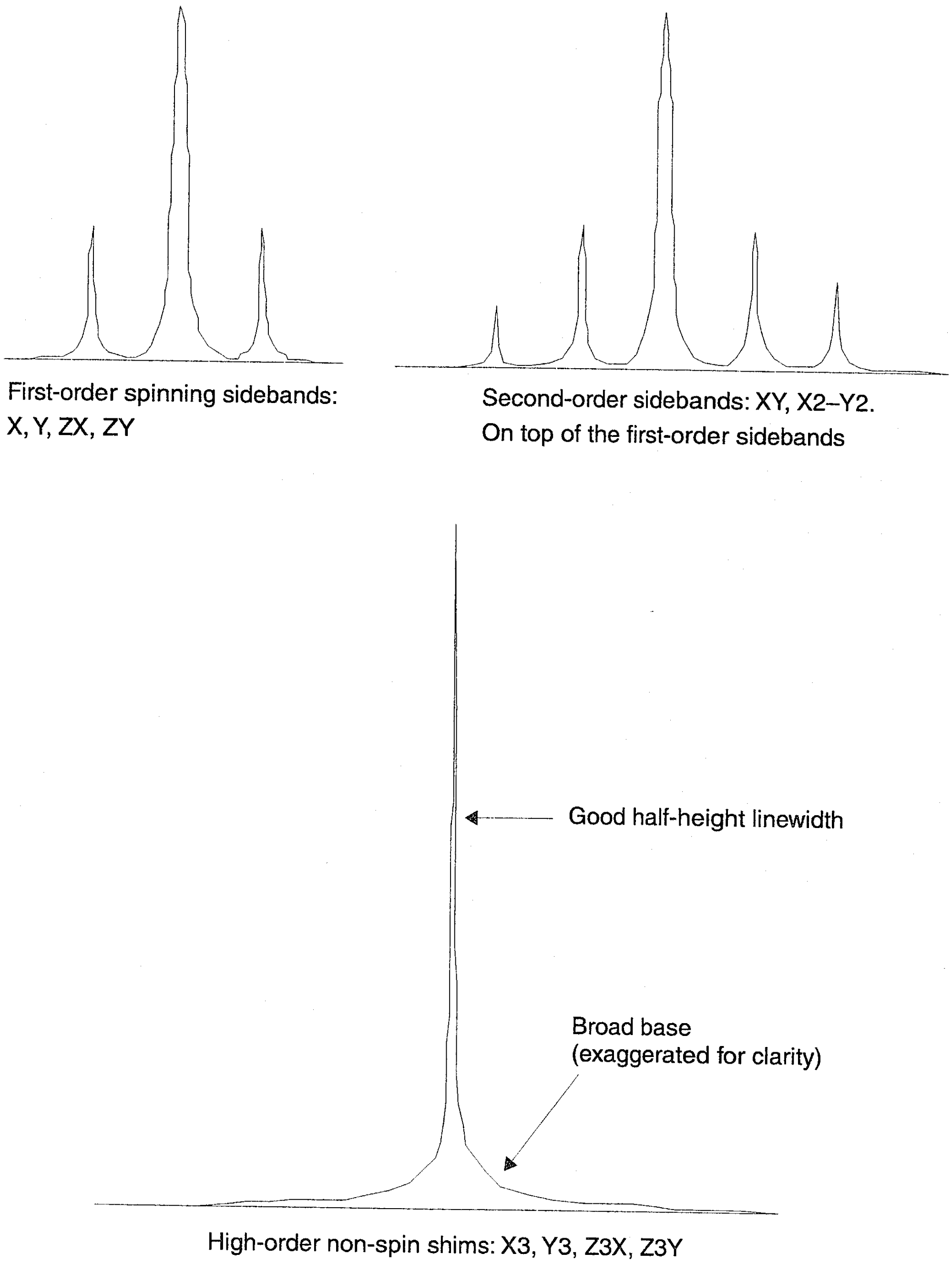

Figure 10. Effects of non-spin shims

Summary of Shim Interactions

Table 1 lists some lineshape effects associated with shims. Note that 13-channel shim systems (`shimset=1`) do not have Z5, Z3X, ZXY, etc., and that 14-channel shim systems (`shimset=10`) have Z5 but do not have Z3X, ZXY, etc.

Table 1. Lineshape effects and their associated shims

Lineshape Effect	*Shims*
Split peak	Z4 and Z1
Asymmetry greater than half-way up	Z2
Asymmetric foot	Z4
Symmetric feet and or low broad base	Z5
Symmetrically broad base	Z3
Spinning sidebands	Low-order radials X1, Y1
Symmetric broad base	High-order radials X3, Y3, etc.

Typical interactions for axial shims:

- Z1 and all other axial shims, to some extent
- Z2 and Z1
- Z3 and Z1
- Z4 and Z2 (with large delta Z4s: Z4 and Z3)
- Z5 and both Z3 and Z1 (Z5 not available on 13-channel shim systems)

Setting Low-Order (Routine) Shims

The following procedure describes how to set the low-order, or routine, shims. You may need to reset Z0 and lock phase if you are making very large changes in the room temperature shims. With this procedure, you should concentrate on improving the symmetry of the main resonance as well as the half-height resonance and line shape.

1. Click on the Connect button in the Acquisition window.
2. Click on the SHIM button and set SPIN to on
3. Adjust the lock level to about 80 if possible.

   Maximize lock level with Z1.

   Maximize lock level with Z1 and Z2. Do this by making a change in Z2 followed by maximizing with Z1 again. Continue to iterate in this manner until you can no longer increase the lock level.
4. Acquire the spectrum.

   If the sample is properly shimmed, the lines should be symmetric.
5. If the lines are not symmetric or unusually broad at the base, refer to Table 1 and the previous sections for which shims to adjust. You should not need to adjust Z3, Z4, or the non-spins for most routine samples.

6. If you do need to adjust Z3, do so by interactively shimming Z1 and Z3 in the manner described in step 3 for Z1 and Z2. Changes in Z3 may affect Z2 so after shimming Z3 maximize Z1 and Z2 again.