# 6. 2nd Order Shimming and High Resolution Check-Out

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## I. 2nd Order Lock Shimming (Match Tuning) on $Z^2$

- Make sure the lock is not saturating. Check by watching that the lock signal increases consistently as increase lock power. Once the lock signal drops or stays steady with increasing power, back off the power by at least 20%.
- Adjust lock level to one square down from the top of the display with LOCK GAIN. Optimize lock level with **z-coarse**, **z-fine**, **$z^2$-fine**, and **z-fine**.
- Change **$z^2$-fine** by 20 units in one direction. Optimize lock level again with **z-fine**. If newly optimized lock level is lower than the previous one, try changing **$z^2$-fine** in the other direction.
- Keep changing **$z^2$-fine** by 20 units in the same direction and optimizing lock level with **z-fine**, until a maximum has been found. Set **z** and **$z^2$** to this maximum setting.
- Lower lock level to one square below top of the display with LOCK GAIN.

## II. High Resolution Check-Out

[*o*-Dichlorobenzene (ODCB) with 3% TMS in $d_6$-acetone is used as High-Res check-out standard.]

### *A. FID Shimming (Line Tuning)*

- After 2nd order shimming (see Section I above), **RJ ACETONE.1DJ** (for $d_6$-acetone); **GS**; **<ctrl> H**; **FT**; **EP**; **<ctrl> R**; **BP**; **<ctrl> B**; phase using **C**- and **D**-knobs; **M** (memorizes phasing); **<ret>** (exits EP); **TR = 2** or **3** (if presently in Job 1); **EP**; find TMS peak, then **R <move cursor> R** to define a window with SW = 150-200 Hz in which TMS peak is positioned approximately half-square off the center; move the cursor to TMS peak; **<ctrl> O** (to set O1 and SW for TMS peak).
- **<esc>** to Acquisition Parameters display. Check **SW = 150-200** Hz, **SI = 16K** (total data size for FT) and **HZ/PT = 0.018-0.024** Hz. [i.e., HZ/PT = 2 SW / SI.]
- **TD = 4K** (total number of data points for FID) and check **AQ = 15** sec. If AQ > 18 or AQ < 13 sec, then **AQ = 15** to automatically set TD. [i.e., AQ = TD / 2 SW.] Remember to use SI > 2 TD for zero-filling!
- **RD = 2-4** (sec); **<esc>** four times (returns to FID/Spectrum display); **GS**; increase Vertical Display to make FID signal fit the entire display; change **$z^2$-fine** by 2 units and optimize FID signal by changing **z-fine** by 2 units at a time at each new $z^2$ setting; keep optimizing until the maximal optimization is reached; **<ctrl> H**.

### *B. Window Set-Up and Acquisition*

- Switch to Job 1 (the original spectrum display of ODCB); **EP**; **R <move cursor> R** to define a 150-200 Hz window which contains all the resonances for ODCB; move the cursor to the center of the display; **<ctrl> O** (to set O1 and SW for this region).
- Make certain that **SW = 150-200** Hz, **SI = 16K**, **HZ/PT = 0.018-0.024** Hz, **AQ = 15** sec, and **RD = 2-4** sec. **AQ > 15** s will actually work better since (resolution) ~ 1/(2*AQ).
- **NS = 8** (scans); **ZG**; **WR <filename>**; transfer FID with **TOPC**
- Or, if desired, store FID and work it up on the AC console as follows:

- After storing FID with **WR <filename>**, **FT**; **EP**; **<ctrl> R**; **BP**; **<ctrl> B**; phase using **C**- and **D**-knobs; **M**; and check if you have split all the peaks into small doublets!

### *C. Lorentzian to Gaussian Line Shape Transformation (Resolution Enhancement)*

- **RE <filename>** (to read FID for ODCB obtained as above); **LB = -HZ/PT / GB** (Note that LB is a negative number; GB is the fraction of the display occupied by the FID when Vertical Display is set to 512; e.g., if HZ/PT = 0.018 and GB = 0.5, then LB = -0.036); **EF** (or EM + FFT on data station); and, phase the spectrum. See also Primer chapter, section on Lorentzian and Gaussian apodization.