

Zero Filling in 1D

NMR SPECTROSCOPY

(Xwinnmr for PC, version 3.5)

on

DPX 200, DPX 300, DRX 500

and

Processing computers

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January 2005.

Version I

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Log in and start xwinnmr.

1. Click on **File** followed by **search**. Select a disk for instance C:. Select one of your own spectra.
2. Type **wrd**↵ this is the command for copying the dataset which is on screen to another disk (home or other place) for permanent storage and at the same time **change the ownership** of the files.

Enter target data set **NAME:** **ZEROFILL**↵ (use your own expname)
 Enter target data set **EXPNO:** **2**↵ (use the expno seen in the top part of the xwinnmr window).
 Enter target data set **PROCNO:** **1**↵ (use the procno seen in the top part of the xwinnmr window).
 Enter target disk unit **DU:** **D:**↵ (if you want to, you can choose M: and the dataset will go to your home directory)
 Enter target user name **USER:** **uio user name**↵ (your own user name)

3. Use **search** to find the ZEROFILL dataset, then **append** and **apply** it to the xwinnmr window and **efp** to Fourier transform it. If the computer you are using does have another plotter attached than the one used under acquisition use **edo** (edit output) to select the new plotter. The data set does regrettfully remember the plotter name connected to the computer used to acquire the spectrum.
4. **efp** and **apk** the spectrum. Expand a sensible part of the spectrum on the screen..
5. Type **eda** to see acquisition parameters. Look for the parameter **TD**. eda parameters can only be changed before the experiments starts.
6. Type **edp** to see processing parameters. Look for the parameter **SI** (size). edp parameters can be changed after the experiment is finished.
7. The **Re** spectrum is presumably consisting of 16k data points. If so the **Im** spectrum has 16k data points. This parameter (data points) is called SI (size). When $SI=TD/2$ no zero filling has taken place.
8. Use **edc** to increase the **procno** (processing numbers) for the following. Change **SI**, either by typing SI in the xwinnmr window or by changing SI in the edp window. Select SI to be 2k, 4k, 8k, 16k, 32k, 64k and 128k. Do an **efp** for each individual SI and watch the result

on the expanded part of the spectrum on the screen. The expansion disappears for each **efp**. Plot if you like with **plot**.

9. When $SI = TD$ you have zero filled once, when $SI = 2TD$ you have zero filled twice. What have you done when $SI = TD/4$ or $SI = TD/8$? Which part of the FID are you using? Why are the spectra looking as they do with low SI ?
10. Zero filling is important in 2D NMR. Another manual will be provided for this purpose. An alternative to zero filling in both 1D and 2D is linear prediction which also will have its own manual.
11. Zero filling is important with wide sweep widths (wide ppm area). The sweep width is connected to the acquisition time (AQ) in such a way that the wider the ppm area is the shorter is the AQ time for a given number of data points (TD). If you do not increase the number of data points when increasing the SW (in hertz or ppm) the AQ drops down. In certain cases the T1 relaxation is not over at the end of the AQ time. This will give bad "wiggles" at the baseline of strong peaks. Zero filling in combination with a WDW (window) function that takes the signal down to zero at the end of the FID (attenuates the signal) can make a bad looking (see above) spectrum better.
12. Change **procno** with **edc**. Open **edp**. Increase **TD** to a higher number. Change **LB** (line broadening) from 0.3 Hz to 3 Hz. Keep EM (exponential multiplication) as the wdw (window function). A separate manual for window functions will appear shortly.
13. **Efp** the FID - watch the difference in appearance!!