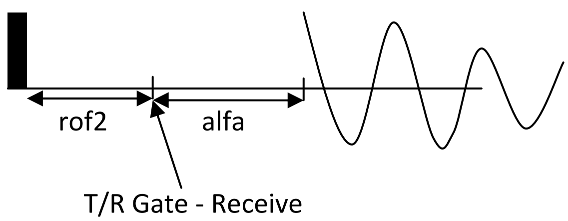
Getting Flat Baseline

A good flat baseline is an essential feature in a NMR spectrum for several reasons. A flat baseline ensures integrity of integrals, reduces t_1 noise in 2D spectrum and in indirect dimensions of nD spectrum. Baseline wobble in a nD dataset will lead to bad quality data.

The baseline of a NMR spectrum depends on several parameters and the experiment. The protocol for controlling the baseline also depends on the vintage of the console. The steps involved for INOVA and VNMRS consoles are different.

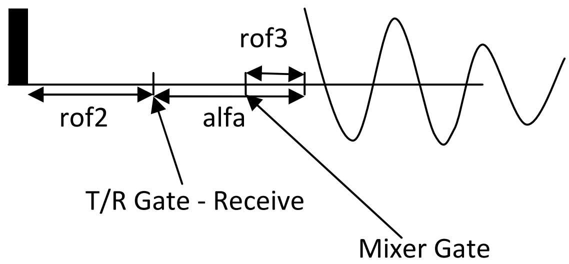
There are few parameters that need to be set properly in order to get flat baseline: they are rof2 and alfa - common to INOVA and VNMRS, rof3 and ddrtc - only for VNMRS. The schematics below help understand these delays.



Schematics for INOVA Console

The first point of the FID is physically observed after a delay of rof2+alfa after the pulse (all timing in μs) while ideally the first point should have been observed at the middle of the pulse. This in turn leads to linear phase difference for various resonances that is reflected as a non-zero lp value when phasing the NMR spectrum. Larger the lp value more the distortion of the resulting baseline. If we minimize the rof2 and alfa delays so that there is no large lp then the rf breakthrough will distort the first few points of FID and will distort the NMR spectrum.

With INOVA spectrometers, a rof2 ~ 4 to 5 μs and alfa ~ 5 to 6 μs will usually give zero lp and flat baseline if dsp='r' or dsp='i'. There are also macros crof2 or calfa that can be used after phasing a spectrum if there are large lp values to get an estimate of rof2 and lp values. Sometimes these macros will give a negative alfa and too short a rof2 value, so as a rule of thumb the above said values could be used. For cold probes – use dsp='i' and qcomp='y' along with the above said values. The dsp algorithm takes into account the total delay and constructs the required points of the FID to make it start from time t=0.



Schematics for VNMRS Console

With VNMRS console, there is a separate parameter ddrtc (μs) that controls the timing. This parameter doesn’t exist by default, create it using the create(‘ddrtc’,’pulse’) command. Usually

ddrtc = rof2+alfa+pw/2 (where pw is the pulse width) and rof2 ~ 28 μs and alfa ~ 5 to 6 μs

The above expression is true only if the sequence is pulse acquire type. If there is a spin-echo type segment (τ -180-τ) just before acquisition then it is enough to set ddrtc=alfa. This, of course, presumes there is no rof2 delay that is uncompensated in the echo segment. The parameter dsp has no effect in VNMRS console and can be set to anything (‘r’,’n’,’i’). The default digital signal processing is done in three stages and there are quite many parameters control them. It is best to leave it in the default mode and worry about it only if extremely large spectral widths are to be acquired. The relatively large value of rof2 is required for good baseline based on the dsp processing done by VNMRS and is used for both romm temperature and cold probes (this value is large enough for cold probes also). The rof3 value is by default 2μs and is part of alfa. Thus alfa should be ≥ 2μs. Do not use the macros crof2 or calfa with VNMRS console.