Absolute Frequency Calculations in VNMR

cgfry: 21.jun.05

sfrq - spectrometer frequency, accurate to all decimal places
VNMR displays a truncated list, but all places can be observed by:

```
spcfrq                          or something like
write('line3','%20.9f',sfrq)
```

dfrq - is handled similar to sfrq

These parameters can be used in calculations (in macros) without concern; complete accuracy is carried throughout.

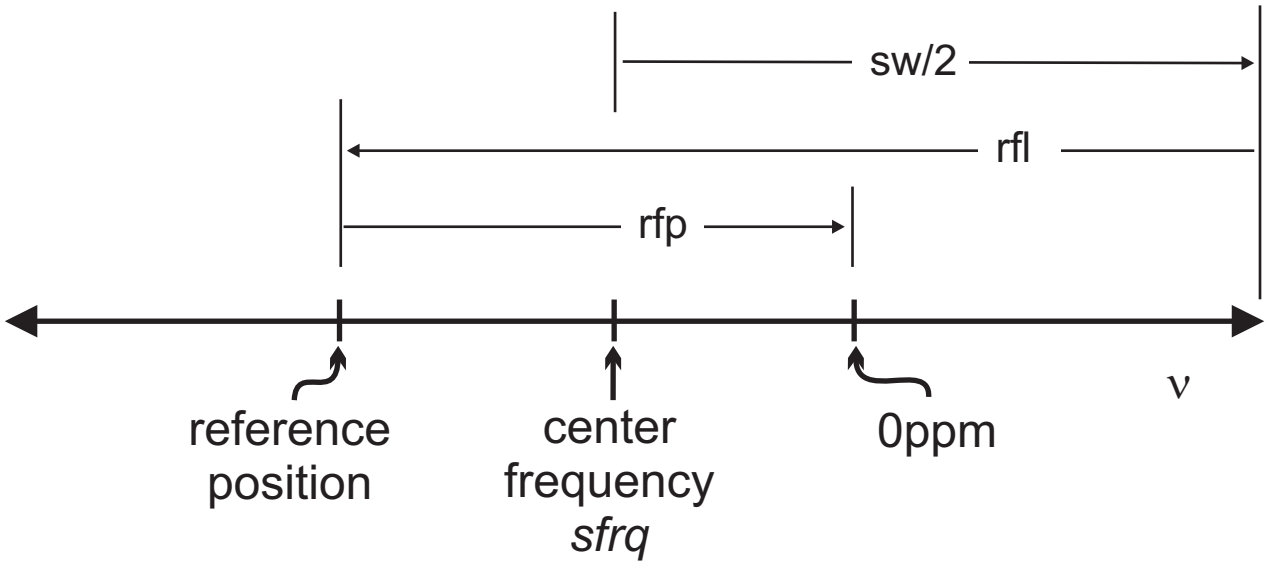
tof - a parameter that makes changing sfrq simple
tof has no other value or property: change it by +105 Hz, and sfrq will increase by 105 Hz. tof is therefore not involved in absolute frequency calculations.

rfl - the frequency from the right edge of the spectrum to the reference line (as described by rfp)

rfp - the frequency of the reference position to 0 ppm; e.g., if use residual water as reference at 4.7ppm (not recommended)
rfp = 4.7p = 2821 Hz (@600.13MHz)

So, absolute frequency of 0 ppm line would always be:

```
absfrq = sfrq*1e6 - sw/2 + rfl - rfp
```



Varian introduced two new parameters in vnmr6.1c:

reffrq - most of the time, reffrq≡absfrq from the previous page

refpos - almost always set =0 (easiest if rfp is also =0)

The indirect dimension in a 2D spectrum follows directly from the previous discussions:

homo2d (e.g., gcosy): reffrq1=reffrq, rfl1=rfl, etc. assuming squared axes have been used.

hetero2d (e.g., hsqc): reffrq1 = dfrq*1e6 - sw1/2 + rfl1 - rfp1

I (cgf) do not recommend the use of the setref macro, except for initial setup purposes. The macro is very hard to read, and is obtuse in some equations used.

I (cgf) also do not recommend the use of the vnmr command setfrq, as it involves calculations that Varian does not document sufficiently to really understand. I have replaced insidences of its use in macros in the UW-Chem facility (e.g., in go_HSQCAD).