Heteronuclear broadband decoupling (Vnmrj 3.2)

E. Alvarado, U of Michigan, 08/23/2013

NMR spectra can be simplified with the application of heteronuclear broadband decoupling. This is normally the default with ^{13}C and ^{31}P spectra where all protons are decoupled. For other spectra, proton decoupling may or may not have been enabled in the standard parameters.

The ^{1}H NMR spectra of protonated boron compounds usually exhibits multiple broadened resonances due to coupling to boron. Boron exists as two isotopes, ^{10}B and ^{11}B with natural abundances of 19.6 and 80.4%, respectively. A proton (or a carbon!) coupled to a boron will show up as the sum of a 1:1:1:1 quartet and a 1:1:1:1:1:1:1 septet in a 4:1 intensity ratio due to coupling to ^{11}B with spin I=3/2; and to ^{10}B with spin I=3. Furthermore, because both nuclei are quadrupolar, boron-coupled proton or carbon resonances are also broadened by quadrupolar relaxation.

Proton NMR spectra of boron compounds can be simplified with the application of ^{11}B decoupling. In decoupled spectra the signals of protons coupled to ^{11}B appear as singlets while those coupled to ^{10}B remain as broad septets with a low intensity of only 20% of the total proton.

The macro `UMsetbbdec` sets up a Wurst-40 adiabatic decoupling scheme that is effective over large spectral widths like those common in many nuclei. `UMsetbbdec` uses three arguments as follows. The first two define the boundaries, in ppm, of the region to decouple and the third is the maximum coupling constant to decouple. For example, to decouple B11 from 80 to 10 ppm with a maximum J of 150 Hz type: `UMsetbbdec(80, 10, 150)`. For more information, read the manual page for `UMsetbbdec`; type `man('UMsetbbdec')`.

To acquire a proton spectrum with heteronuclear decoupling, proceed as follows.

1. Load parameters for proton and enter the nucleus to be decoupled in the decoupler channel, for example `dn='B11'`.
2. Make sure the probe is tuned to both proton and the nucleus of interest.
3. Type `UMsetbbdec(ppm1, ppm2, J)`; for example `UMsetbbdec(80, 10, 150)`.
4. Start the acquisition.

To acquire a X spectrum (C13, P31, etc) with proton decoupling the standard parameters are ready to use but proton decoupling may not be enabled. Make sure it is enabled in the parameter panel Acquire > Defaults. In this panel you also have the choice to have NOE or not. Keep in mind that nuclei with negative magnetogyric ratios like N15, Cd113, Si29, Sn119 develop negative Overhauser enhancements that reduce the signal intensity instead of enhancing it.

When the proton spectrum spreads over more than 10 ppm, like in the case of metal hydrides, the default decoupling scheme (Waltz-16) is not enough. In those cases use `UMsetbbdec` for proton decoupling (`dn='H1'`) as described above.

Decoupling of fluorine can also be accomplished with `UMsetbbdec` as described above. Set `dn='F19'`.

Simultaneous decoupling of both proton and fluorine is described in a separate document (*Fluorine Experiments*).