DEPT and APT experiments (vnmrj 2.2)

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DEPT (Distortionless Enhancement by Polarization Transfer) and APT (Attached Proton Test) experiments are routinely used to help assign ^{13}C spectra. DEPT-135 yields spectra where quaternary carbons are absent; methylene carbons have negative intensities; and methine and methyl carbons are positive. On the other hand, APT yields spectra where both quaternary and methylene carbons are negative, and methine and methyl carbons are positive. There is a modification to the DEPT-135, called DEPTQ-135, that will also show quaternary carbons with negative phase. DEPT experiments can also be run in full editing mode to provide a set of 4 spectra with only C, CH, CH_2 and CH_3 groups each.

Of the two, DEPT is more sensitive and usually preferred.

On modern instruments equipped with indirect detection probes, an alternative experiment is an HSQC (or a gHSQC, gHSQCAD, or gc2hsqc) with multiplicity editing. These experiments not only are more sensitive than DEPT or APT, but they also provide one-bond carbon-proton correlations in addition to multiplicity information. More information is provided in the writeup *Two-dimensional experiments with vnmrj 2.2*.

APT

Acquisition

1. In the main menu select **Experiments > Setup NEW parameters to do... 13C-1H Multiplicity Determination > APT**.

2. Select a solvent (**Start** panel) and lock/shim as usual.

3. In the **Acquire, Defaults** panel change the **Spectral Width** and **Number of scans** if desired.
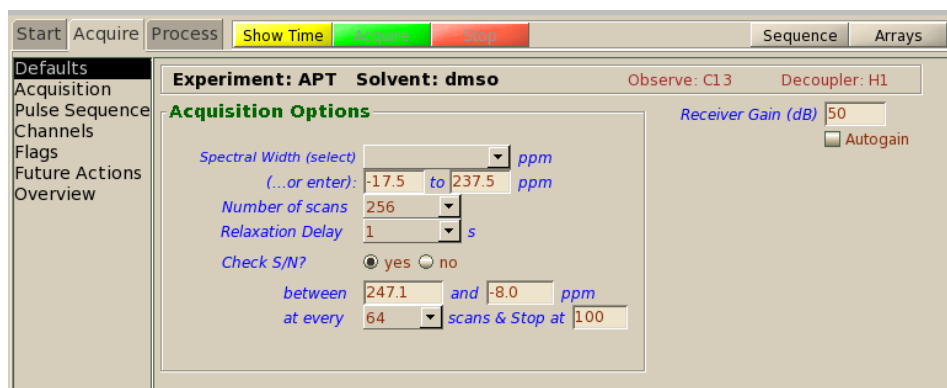
4. If **Check S/N?** Is enabled, the signal to noise ratio in the region indicated will be measured every given number of scans and the acquisition will stop when it reaches the number specified.

Processing and plotting

Since this is a single 1D experiment, it is processed and plotted as usual. Phase the spectrum so that a known peak has the expected sign.

DEPT

Acquisition

1. In the main menu select **Experiments > Setup NEW parameters to do... 13C-1H Multiplicity Determination > DEPT**.

2. Select a solvent (**Start** panel) and lock/shim as usual.

3. In the **Acquire, Defaults** panel change the **Spectral Width** and **Number of scans** if desired.
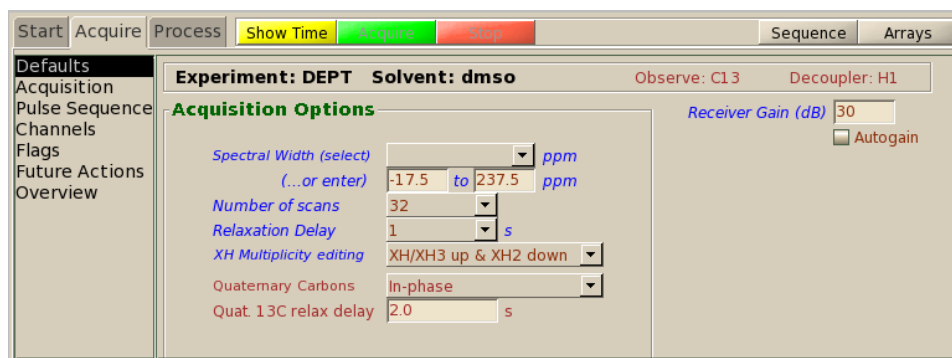
4. For a single DEPT-135 spectrum select **XH/XH3 up & XH2 down** in the **XH Multiplicity editing** drop down menu and **Suppress** in the **Quaternary Carbons** menu (or choose **Antiphase** for a DEPTQ-135).

    For the set of 4 edited spectra (will take 4 times longer) select **Full Edit** in the **XH Multiplicity editing** drop down menu and **Enable editing** in the **Quaternary Carbons** drop down menu.

    For a DEPT-45 (all protonated carbons equally enhanced, useful for 1D spectra of nuclei with negative magnetogyric ratios; for example for ^{15}N or ^{29}Si), select **No Edit** in the **XH Multiplicity Editing** and **Suppress** in the **Quaternary Carbons** menu.

    For a DEPT-90, where only methine carbons will show, select **XH only** and **Suppress**.

5. Click **Acquire** to start the acquisition.

Processing and plotting

Single-spectrum DEPT experiments are processed and plotted as usual for 1D experiments. Use a peak of known multiplicity to phase the spectrum correctly.

To transform edited experiments, click **Transform all** and **Full Edit** in the **Process, Default** panel, and **Plot Spectrum Array** in the **Plot** panel to plot it.