Absolute δ Referencing for Nuclei other than ^{1}H
Using the "xref" macro in VNMR

For quite some time, methods that reference "X" nuclei (i.e. ^{13}C, ^{31}P, ^{29}Si, ^{11}B, ^{15}N, ^{19}F, ^{195}Pt) to their accepted zero PPM reference compound, which use the absolute NMR frequence of TMS in the ^{1}H spectrum have been widely applied. Recently, the IUPAC has released official documentation for the application of absolute, indirect chemical shift referencing of all common "X" nuclei {R. Harris, et.al, *Pure Appl. Chem.,* **80**(1), 59-84 (2008) }. The advantage of this method is that the chemical is referenced absolutely to zero-ppm for ^{1}H, making it unnecessary to use any cumberson internal/external reference compound for your X-nucleus NMR spectrum.

A macro called "xref" has been installed on all of the Varian instrument computers and workstations, which allows one to absolutely reference any X-nucleus spectrum using its associated ^{1}H spectrum that has been correctly referenced to TMS. To use this macro, you must acquire (and save, prefereably) a ^{1}H NMR spectrum when the X-nucleus spectrum is acquired. The xref macro was originally written by David Live, and contributed to the Varian User Library by Bev. Ostrowski at the University of Minnesota, and updated by Charlie Frye, and the University of Winconsin Madison.

How to use the xref macro command:

1. On the NMR spectrometer:
    a. Join EXP:1 by typing **jexp1 <Ret>**, and acquire a ^{1}H NMR spectrum. Reference this spectrum to TMS using normal methods (i.e. residual solvent resonance). You should save this spectrum.
    b. Join EXP:2 by typing **jexp2 <Ret>**, and setup/acquire your X-nucleus spectrum (i.e. ^{31}P, ^{11}B, …etc.). At any time (even while the acquisition is proceeding), you can type **xref <Ret>**, and you will be asked "Enter Experiment Number containing the 1H NMR spectrum". If you did step (a) above in EXP:1, you would enter the number **1 <Ret>**. You should see a message indicating that your spectrum is referenced, and the compound that is considered "zero" for that nucleus.
    c. When you save this spectrum (in EXP:2), it will be correctly referenced according to the IUPAC standard frequency ratios for your X-nucleus. If you open this in any NMR software, it should be correctly referenced to zero, and require no further referencing/calibration.

2. On a Datastation (after the fact): This requires that the ^{1}H spectrum for the sample has also been saved when the X-nucleus spectrum was acquired.
    a. Join EXP:1 by typing **jexp1 <Ret>**, load the ^{1}H NMR spectrum of the compound, and type **wft**.
    b. Reference this spectrum to TMS using normal methods (i.e. residual solvent resonance).
    c. Join EXP:2 by typing **jexp2 <Ret>**, and load your X-nucleus spectrum (i.e. ^{31}P, ^{11}B, …etc.).
    d. Type **xref <Ret>**, and you will be prompted to enter the Experiment Number containing the ^{1}H NMR spectrum. Enter the number (**1 <Ret>** in this example where the 1H spectrum is in EXP:1).
    e. You should resave this spectrum (either with a new filename or the same filename by typing **resave <Ret>**) after the chemical shift axis is properly referenced.