Delta Tips

NMR data processing software

Delta NMR Software

NMDT_0076

Temperature Calculator

As the thermocouple to measure NMR sample temperature is placed in the vicinity of the NMR tube, not inside the tube, we rather monitor temperature of gas either cooling or heating our NMR sample. For most applications, this approach is perhaps sufficient. However, it is important to report sample temperature more accurately when measuring relaxation times, diffusion coefficients and chemical shifts sensitive to temperature. The **Temperature Calculator** is a tool which allows us to determine actual temperature inside the NMR sample by using a standard sample such as methanol or ethylene glycol. Signals of these standard samples are sensitive to temperature and allow us to determine sample temperature by measuring the difference in chemical shifts of two signals in the spectrum. For example, the temperature calibration formula of ethylene glycol is as follows:

$$T(\mathrm{K}) = -0.39(\Delta\delta)^2 - 100.91(\Delta\delta) + 192.62 + 273.16$$

$\Delta\delta$: the proton chemical shift difference in ppm

Temperature calibration samples :

In the example bellow, we will introduce two calibration samples, methanol and ethylene glycol. It is necessary to use high purity samples of recommended composition.
The chemical shifts of methanol and ethylene glycol decrease at high temperature, because the strength of intramolecular hydrogen bonds decreases with increasing temperature.

Low temperature calibration sample, methanol :

Temperature range: -95℃ to +57℃
Measure the proton chemical shift difference between the CH_3 and OH signals, and calculate actual sample temperature.

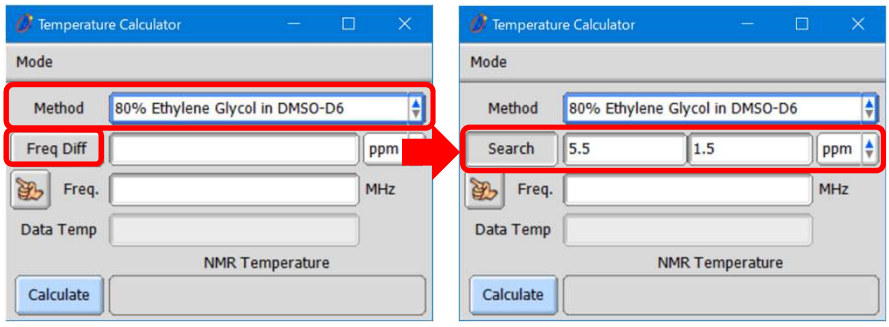
High temperature calibration sample, ethylene glycol :

Temperature range: 0℃ to +143℃
Measure the proton chemical shift difference between the CH_2 and OH signals, and calculate actual sample temperature.

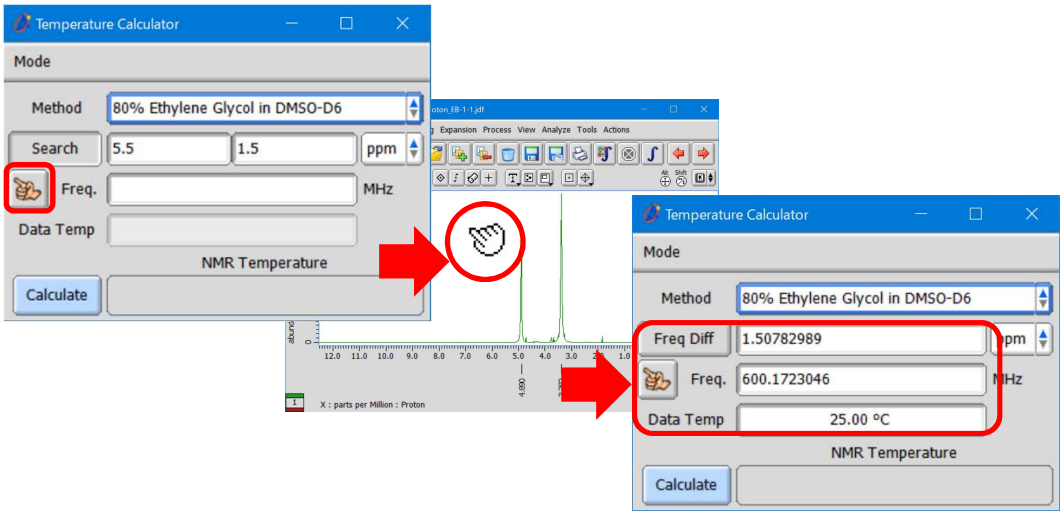
How to use the Temperature Calculator tool :

① Select **Tools**—**Calculators**—**Temperature** in the **Delta Console** window to open the **Temperature Calculator** window.

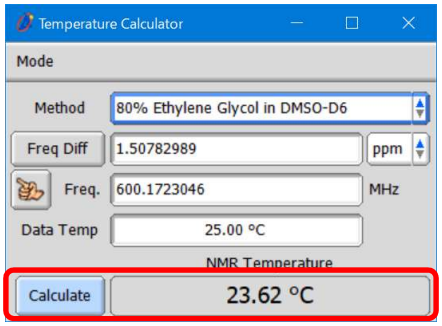
② Select the sample in the **Method** list in the **Temperature Calculator** window. Click the **Freq Diff** Freq Diff button. Note that the **Freq Diff** button has changed into the **Search** Search button and displayed a range of proton chemical shifts in ppm.



③ Click the **Finger** button and select the data of ethylene glycol with the **Finger** cursor as shown below. Note that the tool automatically loaded the chemical shift difference and the proton resonance frequency of the spectrometer from the spectrum.



④ Click the **Calculate** button to display the result. Note that the difference between the preset temperature and the actual temperature inside the sample is approximately 1.4 ℃.



[1] R.E. Hoffman and E.D. Becker, *Journal of Magnetic Resonance*, **176**, 87–98 (2005).