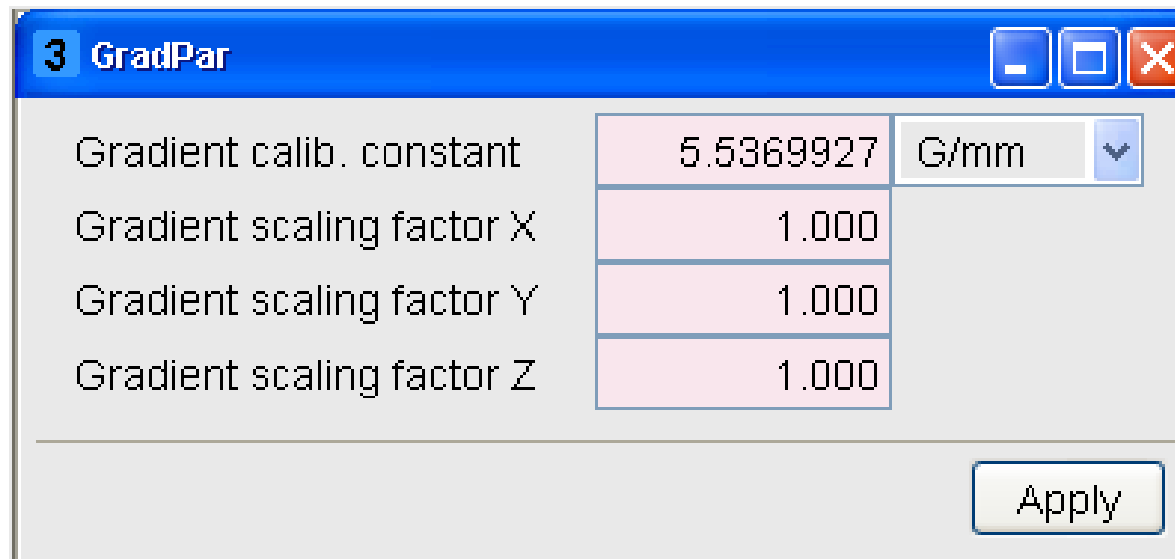


Gradient Calibration



- For the accurate calculation of a diffusion coefficient the maximum gradient strength must be measured and stored in the file <TOPSPINHOME>/conf/instr/gradient_calib.
- This file can be accessed using “**gradpar**”

A screenshot of the "GradPar" dialog box in a software application. The dialog has a blue title bar with the text "3 GradPar" and standard window control buttons (minimize, maximize, close). The main area contains a table with four rows. The first row is "Gradient calib. constant" with a value of "5.5369927" and a unit dropdown menu set to "G/mm". The second row is "Gradient scaling factor X" with a value of "1.000". The third row is "Gradient scaling factor Y" with a value of "1.000". The fourth row is "Gradient scaling factor Z" with a value of "1.000". At the bottom right of the dialog is an "Apply" button.

Gradient calib. constant	5.5369927	G/mm
Gradient scaling factor X	1.000	
Gradient scaling factor Y	1.000	
Gradient scaling factor Z	1.000	

Apply

Gradient Calibration



- **Using Diffusion measurements** – (calibrate g based on a known D)
 - Recommend using the standard doped water sample
 - Diffusion coefficient (D) of D₂O is known (1.872 x 10⁻⁹ m²/s @ 25°C)
 - Diffusion of liquids is highly temperature dependent, so prior temperature calibration is highly recommended.
 - Measure the Diffusion Coefficient (D) of HOD with current calibration
 - For a single axis system (Z only), calculate the corrected Gradient Calibration Coefficient as follows:

$$GCC_{\text{new}} = GCC_{\text{old}} \sqrt{\frac{D_{\text{experimental}}}{D_{\text{literatre}}}}$$

Gradient Calibration



- **Using A Phantom Sample**

- This sample consists of a special plug inserted into the bottom of an NMR tube and immersed in H₂O.
 - Otherwise a limiting volume (shigemi) NMR tube can also be used.
- The gradient strength is calibrated for 5% gradient amplitude and extrapolation to 100% amplitude to give the maximum gradient output.
- Less sensitive to temperature dependencies, but more sensitive to operator judgment

Gradient Calibration



Parameters for Gradient Calibration Using Phantom

Sample: Phantom sample in H₂O

Pulse Program: calibgp

F1 = ¹H P1 and PL1 for 90 deg hard ¹H pulse

AQ ~ 20 ms (adjust **TD** (~4k) and **SWH** (~125ppm) accordingly)

Length of first gradient: **GR_LEN** = 0.5 * **AQ**

Length of second gradient : **AQ**

D21: 200u

Gradient strength

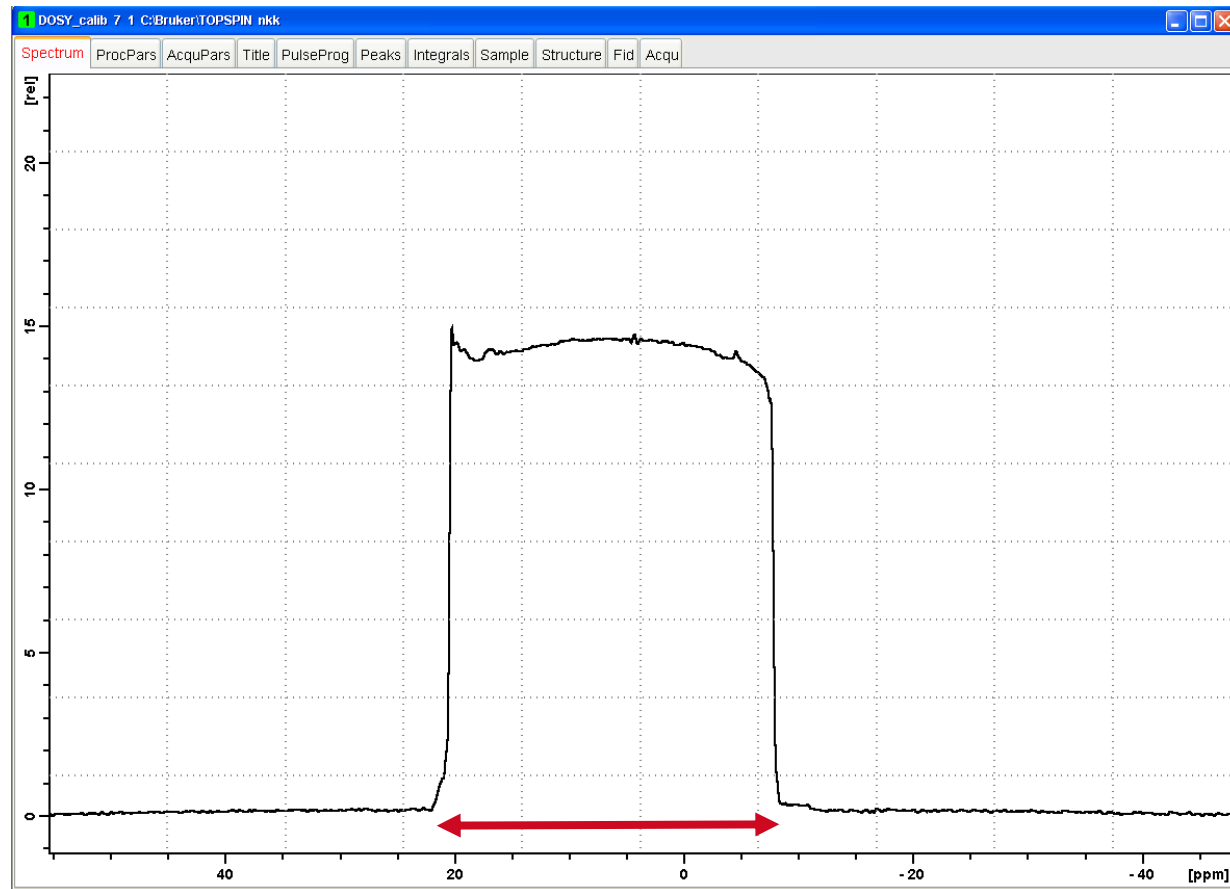
Gpz1 = 5, **gzy1** = 0, **gpx1** = 0 for z-axis calibration

Gpz1 = 0, **gzy1** = 5, **gpx1** = 0 for y-axis calibration

Gpz1 = 0, **gzy1** = 0, **gpx1** = 5 for x-axis calibration

Process data with **WDW** = sine and **SSB** = 0 (sinm, ft & mc)

Gradient Calibration



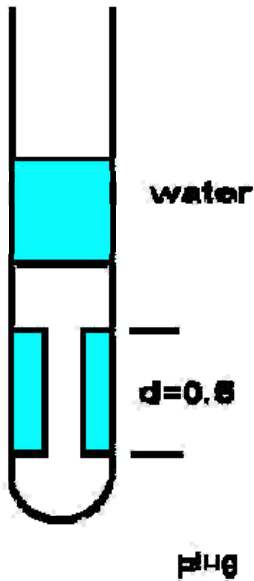
After acquisition and processing measure the width of the hump at the baseline in Hz. This is the value of $\Delta\omega$ which can be plugged into the appropriate equation.

Gradient Calibration



Gradient Strength Calibration Using Phantom

For z-axis gradient



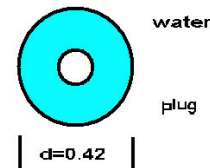
$$\Delta\omega = \gamma G_z \Delta z$$

$$G_z = \Delta\omega / \gamma \Delta z$$

$$\Delta z = d$$

$$G_z = \frac{\Delta\omega \text{ (kHz)}}{[4.258][d \text{ (cm)}]}$$

For x- & y-axis gradients



$$\Delta\omega = \gamma G_x \Delta x$$

$$G_x = \Delta\omega / \gamma \Delta x$$

$$\Delta x = d$$

$$G_x = \frac{\Delta\omega \text{ (kHz)}}{[4.258][d \text{ (cm)}]}$$