Guidelines for Acquisition of UWNMR spectra using WCPMG

Recommended sample: glycine HCl

Field of choice: 14.1 T

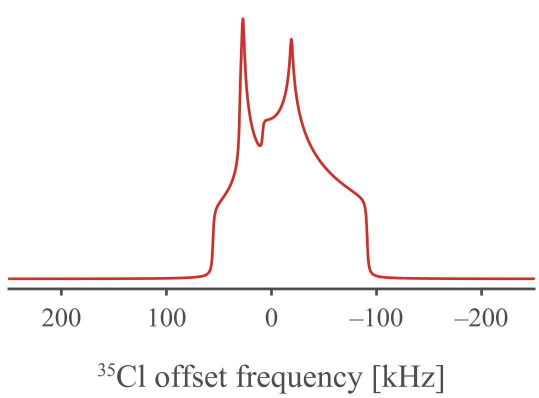
^{35}Cl (S = 3/2) Larmor frequency: 58.78 MHz

NMR Parameters

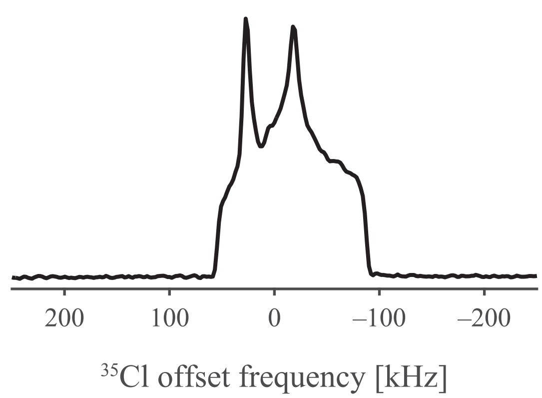
C_Q (MHz)	6.5
η_Q	0.6
δ_{iso} (ppm)	101
Ω (ppm)	100
κ	0.3

Total pattern breadth at 14.1 T: 2480 ppm / 145 kHz

Ideal simulated pattern

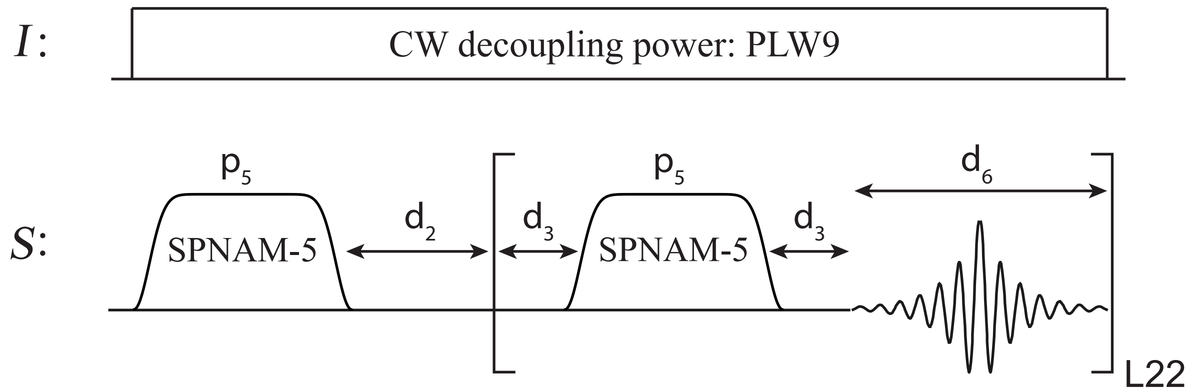


Experimental spectrum



Experimental Parameters	Bruker notation	Value
Pulse sequence file name	–	wcpmg.jk
Number of Transients	NS	16
Recycle Delay (s)	D1	1
Dwell Time (μs)	DW	1
Number of Meiboom-Gill loops, N	L22	50
Spin Echo Length, τ_{SE} (μs)	D6	300
Acquisition Time (ms)	AQ	18.9
Ring-Down Delay, τ_{dead} (μs)	D3	10
WURST-B length, τ_B (μs)	P5	50
WURST-B Sweep width, Δ_B (kHz)	SPNAM-5	300
WURST-B Amplitude, $\nu_{1,B}$ (kHz)	SPW5	10.9
WURST-C length, τ_C (μs)	P5	50
WURST-C Sweep width, Δ_C (kHz)	SPNAM-5	300
WURST-C Amplitude, $\nu_{1,C}$ (kHz)	SPW5	10.9
^{1}H CW Decoupling RF Power (kHz)	PLW9	50
Spectrum Width (kHz)	SW	1000

Pulse Sequence Schematic with Bruker variable notation:



Key points:

1. Generally, the WURST-B and -C pulses are identical ($\Delta_B = \Delta_C$, $\tau_B = \tau_C$, and $\nu_{1,B} = \nu_{1,C}$).

2. The optimal value for Δ_B and Δ_C is *ca*. 1.5 to 2.0 times the pattern breadth (*NB:* this parameter is field dependent).

3. The optimal values for $\nu_{1,B}$ and $\nu_{1,C}$ are given by the following expression: $\nu_{1,B/C} \approx \frac{0.26\sqrt{R}}{S+1/2}$ where R is the rate of the WURST pulse defined as the ratio of the sweep width to the pulse length: $R = \Delta_{B/C}/\tau_{B/C}$

4. The SNR and resolution of experimental spectra acquired with WCPMG are related directly and indirectly, respectively, to R.

Suggested references:

(1) O'Dell, L. A.; Schurko, R. W. *Chem. Phys. Lett.* **2008**, *464*, 97–102.
(2) O'Dell, L. A.; Rossini, A. J.; Schurko, R. W. *Chem. Phys. Lett.* **2009**, *468*, 330–335.
(3) MacGregor, A. W.; O'Dell, L. A.; Schurko, R. W. *J. Magn. Reson.* **2011**, *208*, 103–113.
(4) Schurko, R. W. *Encycl. Magn. Reson.* **2011**.
(5) Schurko, R. W. *Acc. Chem. Res.* **2013**, *46*, 1985–1995.
(6) O'Dell, L. A. *Solid State Nucl. Magn. Reson.* **2013**, *55–56*, 28–41.
(7) Veinberg, S. L.; Lindquist, A. W.; Jaroszewicz, M. J.; Schurko, R. W. *Solid State Nucl. Magn. Reson.* **2017**, *84*, 45–58.
(8) Koppe, J.; Hansen, M. R.; Hansen, M. R. *J. Phys. Chem. A* **2020**, *124*, 4314–4321.