^{13}C NMR Spectra with ^{1}H WALTZ Decoupling

1. Introduction

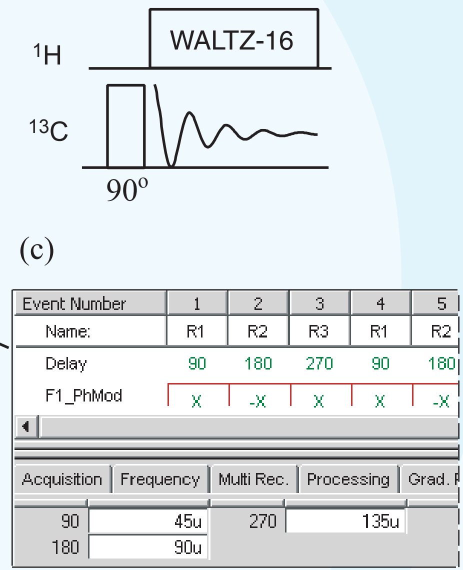
The simplest decoupling scheme is the continuous wave (cw) irradiation at a single decoupling frequency. Though effective at the decoupling frequency, cw decoupling can not cover a wide frequency range. It is often desirable to provide decoupling that is effective over the whole range of a spectrum. Demonstrated herein is the WALTZ-16 sequence for this purpose,

$$\text{WALTZ-16} = RR\bar{R}\bar{R}\ \bar{R}RR\bar{R}\ R\bar{R}\bar{R}R\ \bar{R}\bar{R}RR, \qquad \text{(Eq. 1)}$$

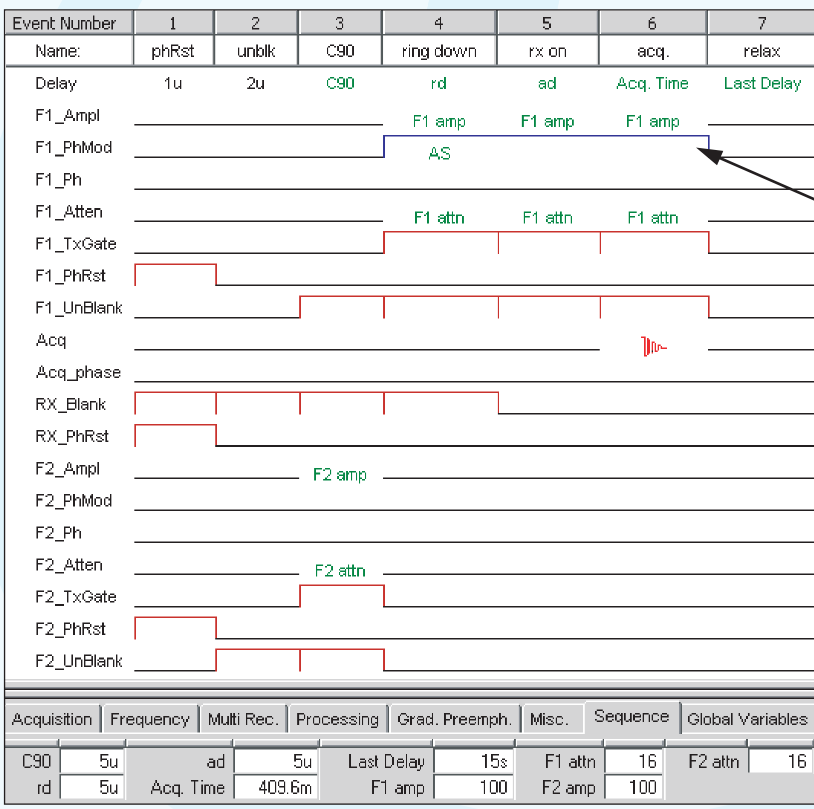
where the basic element, R equals $90^o{}_x 180^o{}_{-x} 270^o{}_x$. If all pulses are expressed as multiples 90^o, R equals $1\bar{2}3$ (hence the name WALTZ). In this example, the WALTZ-16 sequence is implemented as a subsequence. We demonstrate how to use the Asynchronous function to merge a subsequence into the main sequence. It significantly simplifies the pulse editing and appearance of a sequence is more straight forward.

2. Pulse sequence

(a)



(b)



(c)

Fig. 1. (a) The pulse sequence with a single ^{13}C excitation pulse and ^{1}H decoupling during acquisition. (b) The sequence in the NTNMR sequence editor. F1 is the ^{1}H and F2 is the ^{13}C channel. (c) The WALTZ -16 sequence in the NTNMR sequence editor (partial view). It is loaded into the main sequence (b) by the Asynchronous function.

3. Experiment

Sample:	Ethanol
Spectrometer:	7 Tesla Magnet with Tecmag HF3 discovery
Probe:	Nalorac D300-5 OWB 5mm ^{1}H/^{13}C Switchable probe
^{1}H decoupling field:	5.6 kHz (90^o = 45 μs @ 800 mW)
^{13}C 90^o pulse:	5 μs (@ 250 W)

3. Experiment (continued)

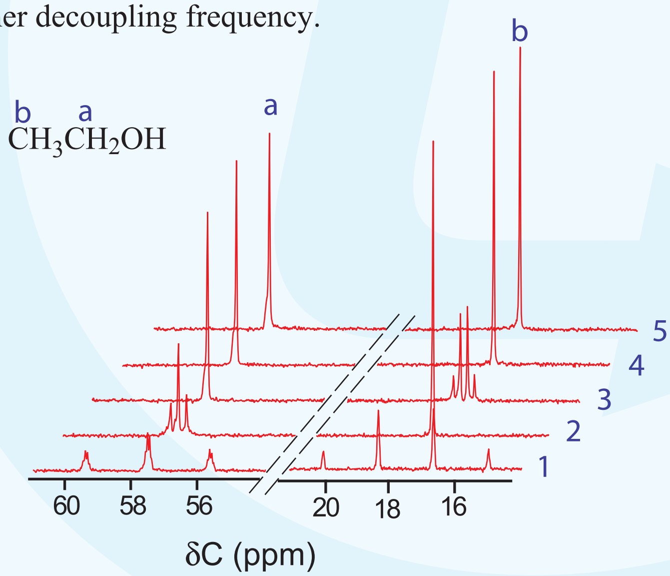
SW +/-: ± 6.5kHz
Last Delay: 2s
Scans 1D: 8

Set up the proton WALTZ-16 sequence (Fig. 1c):
Calibrate the ^{1}H 90º pulse width. After that, set the resulting power level in the lines "F1_Ampl" and "F1_Attn" of the main sequence (Fig. 1b). In a new NTNMR sequence editor widow, set the pulse widths in the "Delay" line, and set the phases in the "F1_Mod" line according to Eq.1. Finally, save the sequence as a sequence file, e.g., WALTZ-16.tps, using the "Save Sequence As..." command.

Load the proton WALTZ-16 sequence into the main sequence:
On the "F1_PhMod" of the main sequence editor window (Fig.2b), left-click on the event during which the WALTZ-16 sequence should start. A pop-up menu appears. Select the option "Add Asynchronous Start" and then select WALTZ-16.tps in the File Open dialog box. To define the end of the decoupling, left-click the cell where the WALTZ sequence shall stop, and select "Add Asynchronous Stop" in the pop-up menu.

4. Results

Figure 2 shows the ^{13}C C_2H_5OH spectra with varies ^{1}H decoupling schemes for comparision. With no ^{1}H decoupling (Spectrum 1), the spectrum shows a quartet for CH_3 and a triplet for CH_2 (1). With cw decoupling and the frequency set to H_a (Spectrum 2), or H_b (Spectrum 3), the respective other carbon is only partially decoupled. Using the WALTZ-16 sequence and the frequency set to $^{1}H_a$ (Spectrum 4), or $^{1}H_b$ (Spectrum 5), the spectra indicate that WALTZ provides sufficient proton decoupling for both lines at either decoupling frequency.



Spectrum	Dcp* method	Dcp freq.
1	- (no dcp)	-
2	cw	f (H_a)
3	cw	f (H_b)
4	WALTZ-16	f (H_a)
5	WALTZ-16	f (H_b)

(*: Dcp = Decoupling)

Fig. 2. The ^{13}C C_2H_5OH spectra with varies proton decoupling schemes acquired with the sequence shown in Fig. 1.

5. References

1. A. J. Shaka, J. Keeler and R. Freeman, *J. Magn. Reson.* **1983***, 53,* 313.
2. E. D. Becker, "High Resolution NMR", 3rd Ed. Academic Press, 2000, p242.