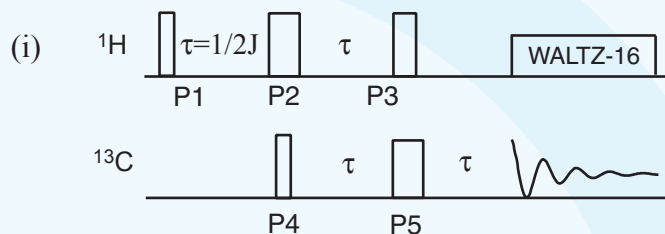


1. Introduction

The Distortionless Enhancement by Polarization Transfer (DEPT) sequence uses a polarization transfer from protons to a nucleus X over one chemical bond to increase the signal strength. The experiment is also used for distinguishing CH₃, CH₂ and CH groups. For molecules containing a large number of carbon atoms it is desirable to generate separate subspectra for CH₃, CH₂ and CH groups. Described here is the sequence editing procedure to obtain three subspectra. This example demonstrates the basic procedure of double resonance 1D NMR data acquisition and processing on Tecmag spectrometers.

2. Pulse sequence



(ii)

Pulse width and phase cycle:

P1 (H90°): 0

P2 (H180°): pH2 = 0, 2, 1, 3.

P3 (H45°/90°/135°): pH3 = (1)₄, (3)₄.

P4 (C90°): pHC1 = (0)₈, (1)₈, (2)₈, (3)₈.

P5 (C180°): pHC2 = (0, 2)₄, (1, 3)₄.

Receiver: phrx = (1)₂, (3)₄, (1)₂, (2)₂, (0)₄, (2)₂, (3)₂,

(1)₄, (3)₂, (0)₂, (2)₄, (0)₂.

(pH2, pH3, pHC1, pHC2, phRX are 1D phase tables.)

All tables are in 4 step mode.)

WALTZ-16 = RR \bar{R} \bar{R} \bar{R} RR \bar{R} RR \bar{R} \bar{R} RR \bar{R} \bar{R} ,
R = 90_x180_{-x}270_x

Event Number	1	2	3	4	5
Name:	R1	R2	R3	R1	R2
Delay	90	180	270	90	180
F1_Ampl					
F1_PhMod	X	-X	X	X	-X

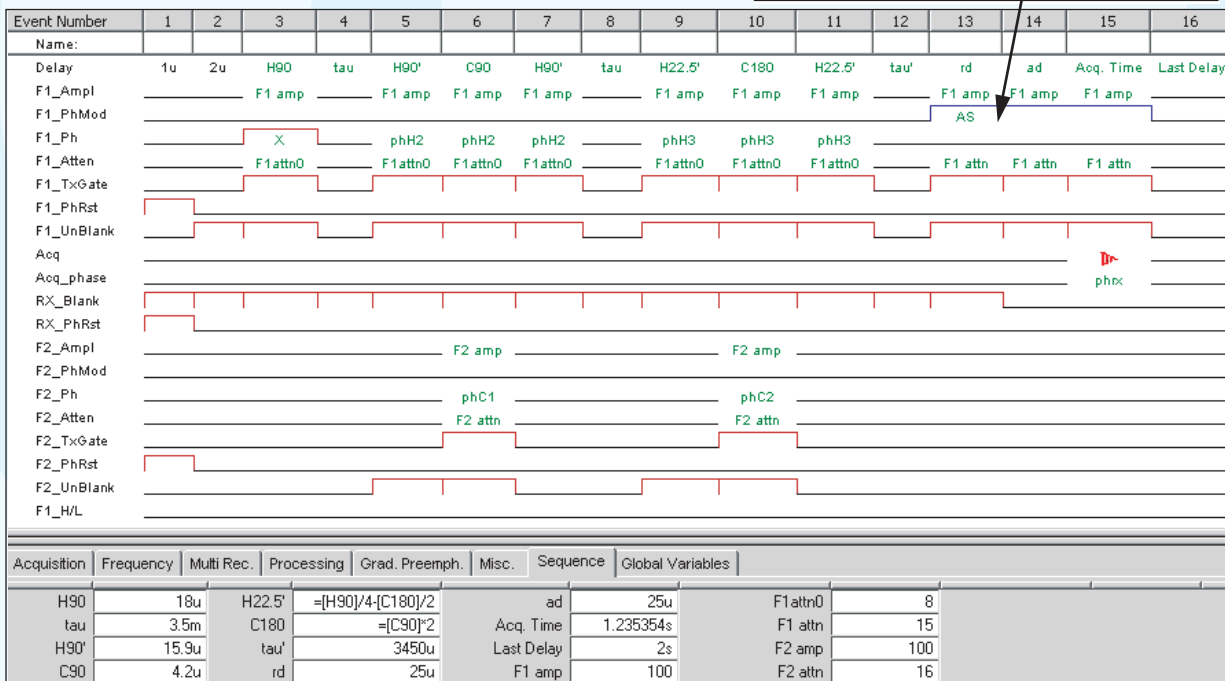
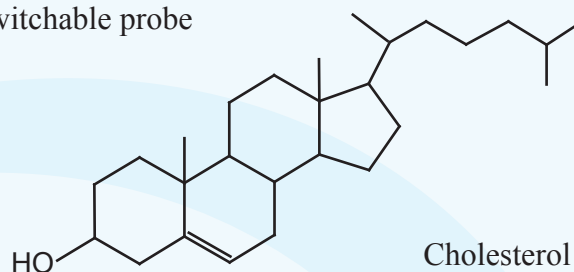


Fig. 1. (i) The editing ¹³C DEPT sequence with WALTZ-16 sequence for ¹H decoupling. (ii) The sequence in the NTNMR sequence editor. Three different pulse widths for P3 (45°, 90° or 135°) yield in three spectra: a) P3 = 45°, all peaks are positive; b) P3 = 90°, only the peaks of CH groups appear; c) P3 = 135°, the peaks of CH and CH₃ are positive, and those of CH₂ are negative.

3. Experiment

Sample: Cholesterol in CDCl₃ (50mg/ml)
 Spectrometer: 7 Tesla Magnet with Tecmag HF3 discovery
 Probe: Nalorac D300-5 OWB 5mm ¹H/¹³C Switchable probe
¹H hard pulse: 13.9 kHz (90° = 18 μs @ 5W)
¹H decoupling field: 5.6 kHz (90° = 45 μs @ 800 mW)
¹³C hard pulse: 59.5 kHz (90° = 4.2 μs @ 250 W)
 τ: 3.5 ms (= 1/(2J_{C,H}) = 140 Hz)
 Spectrum width: ± 6.5kHz
 Recycling time: 2s
 Number of scans: 512



Notes:

1. Before editing the sequence (Fig. 1b), calibrate the 90° pulse widths of ¹H and ¹³C using the nutation experiment (see note, "One Pulse Experiment and Pulse Calibration").
2. Set up the WALTZ sequence according to the note, "¹³C NMR Spectra with ¹H WALTZ Decoupling".
3. The center of pulses P2 and P4 (also P3 and P5) should be aligned. Since P2 > P4 (and P3 > P5) P2 (and P3) have to split into 3 pulses. The delay of P2's (and P3's) middle pulse equals to P4 (and P5), and the delay of both sides is (P2 - P4)/2 [and (P3 - P5)/2]. The middle pulse of P2 (and P3) falls on the same event as P4 (and P5).

4. Results

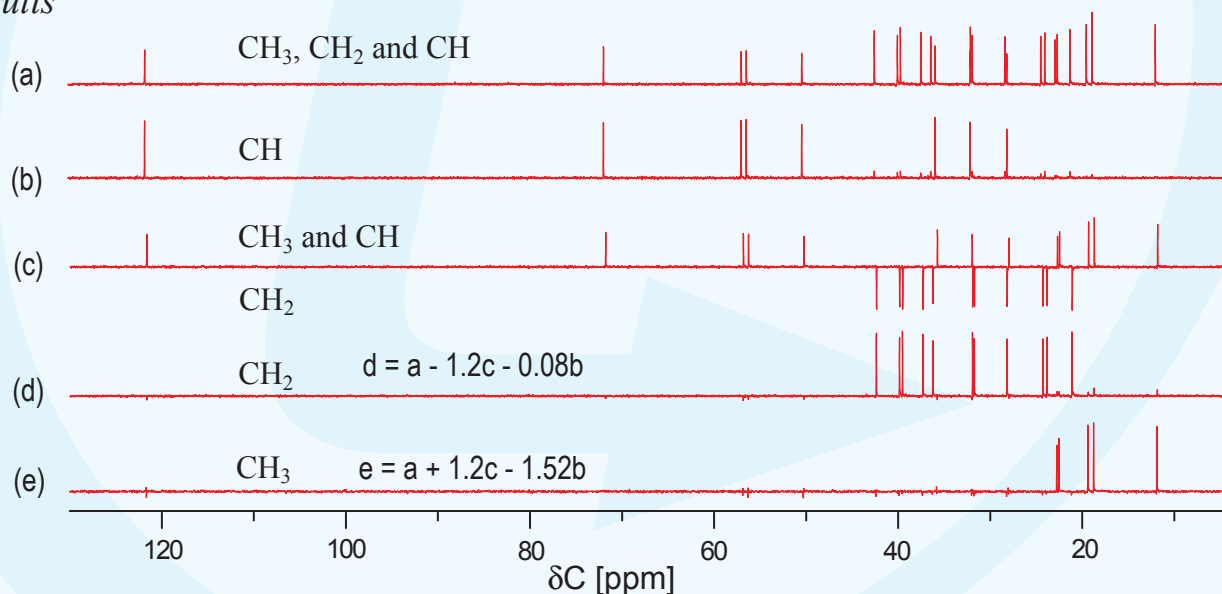


Fig. 2. The Editing DEPT¹³C spectra of cholesterol in CDCl₃. Spectra a, b, and c are correspondent to P3 = 45°, 90°, and 135° in the sequence shown in Fig.1. Spectra d and e are calculated using spectra a, b and c and the equations shown in the figure. The calculation is done by a script, "Editing DEPT".

5. References

1. M.R. Bendall, D.M. Doddrell, D.T.Pegg, *J. Am. Chem. Soc.* **1981**, *103*, 4603-4605.
2. D.M. Doddrell, D.T.Pegg, M.R. Bendall, *J. Magn. Res.* **1982**, *48*, 323-327.
3. S. Braun, H.-O. Kalinowski, S. Berger, "150 and More Basic NMR Experiments", Wiley-VCH, 1999, 183-184.