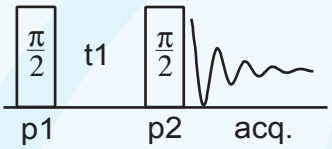
1. Introduction

The COSY (COrrelation SpectroscopY) experiment generates 2D NMR correlation spectra. In the COSY sequence (Fig.1a), the first 90° pulse generates transverse magnetization. The second 90° pulse causes polarization transfer between J-coupled nuclei. For a two spin system with nuclei A and K, two peaks along the diagonal, (ω_A, ω_A) and (ω_K, ω_K), are observed if they are not J-coupled. If they are J-coupled, two additional cross-peaks appear at (ω_A, ω_K) and (ω_K, ω_A). Since coupled protons are typically separated by two or three covalent bonds the chemical structure can be derived from COSY spectra. Described here is a phase sensitive COSY experiment using the TPPI (**T**ime-**P**roportional receiver **P**hase **I**ncrementation) method. With this example, we demonstrate the basic procedure of 2D TPPI phase sensitive NMR data acquisition and processing on Tecmag spectrometers.

2. Pulse sequence

(a)



(b)

1D phase tables:
ph0 (P1): 0, 2, 2, 0, 1, 3, 3, 1.
Ph1 (P2): 0, 2, 0, 2, 1, 3, 1, 3.

2D phase table:
ph1:2 (P1): 0, 1, 2, 3.
(All entries are in 4 step mode.)

2D delay table:
de1:2 (t1): Auto,
Use Dwell Time,
Every Pass.

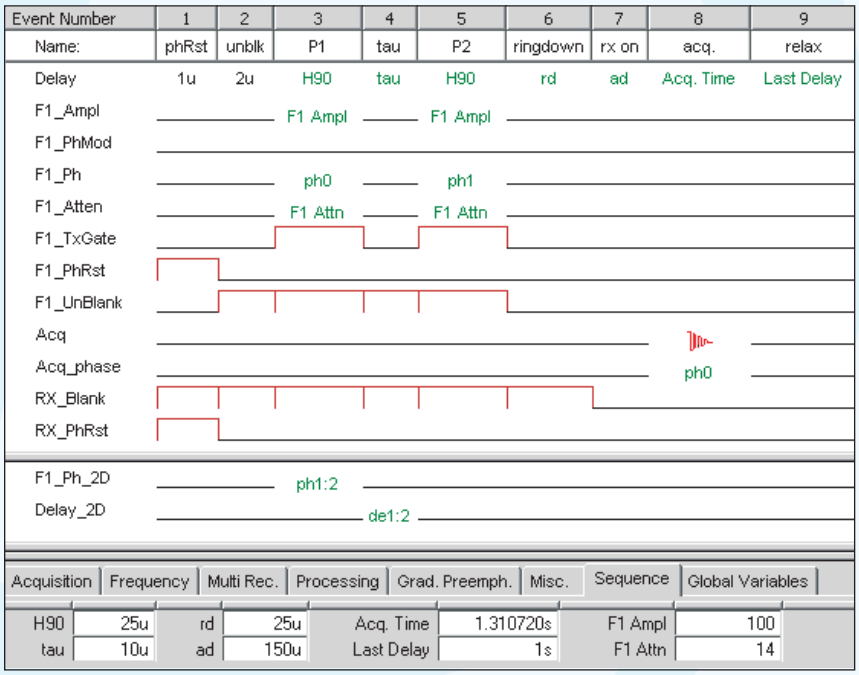


Fig. 1. (a) The pulse sequence for the COSY experiment. (b) The sequence in the NTNMR sequence editor with phase tables set for TPPI method. The 2D phase table "ph1:2" is the phase cycle for P1 according to TPPI. The phase of pulse P1 is sum of the corresponding entries in the 1D phase table, "ph0" and the 2D phase table, "ph1:2". The 2D delay table, "del:2", is used for t1 increments. The t1 values are 1dw, 2dw, ..., ndw, where dw is the dwell time and n is the number in Points 2D.

3. Experiment and results

Sample:	2,3-dibromopropionic acid in benzene-D_6
Spectrometer:	7 Tesla magnet with Tecmag HF3 Discovery
Probe:	Nalorac D300-5 OWB 5mm $^1H/^{13}C$ Switchable probe
90° pulse:	30 µs
SW +/- (1D) :	390.6 Hz
SW 2D:	390.6 Hz

3. Experiment and results (continue)

Dwell time (1D):	1.28 ms
Dwell_2D:	640 µs
Acq. points (and Points 1D):	1024
Points 2D:	1024
Scans 1D:	4

Notes:
The sample is not spun. The magnet is shimmed to ~0.5 Hz line width. If the magnet drift is greater than 0.5 Hz during the experiment, the sample should be locked. Set Dwell_2D = 1/2 Dwell Time for TPPI. For best results, use at least 4 scans in Scans 1D for the 1D phase cycling.

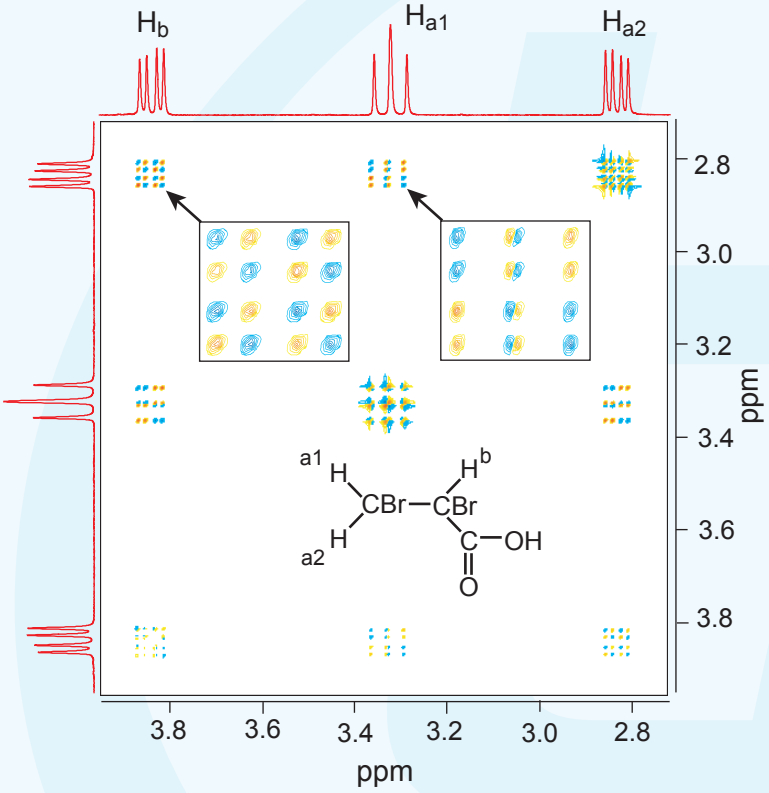


Fig. 2 The phase-sensitive COSY spectrum of 2,3-dibromopropionic acid (Only H_a and H_b are shown). The spectrum is obtained using TPPI method (Fig. 1). A 1D spectrum acquired with a single 90° pulse sequence is shown on the top and left sides.

Data processing:

1. Process 1D data set (The System Phase will be used for 2D processing.).
2. Process the first (t2) dimension of the 2D data set by opening the NDFT window and select: "Use 1D settings", "Fourier Transform", "Use System Phase", "Gaussian GB (1 Hz)", and click "Do it".
3. Process the second (t1) dimension:
   a. to transpose the second into the first dimension, click Commands|Data Manipulation|Transform|Complex;
   b. open the NDFT window and select "Use 1D settings", "Real FT", "No Phasing", "Gaussian GB (1 Hz)", and click "Do it";
   c. to remove the mirror image, click Commands|Data Manipulation| Read Second Half;
   d. to transpose t1 back to the second dimension, click Commands|Data Manipulation| Transform|Complex.
4. To display the processed data, click the 2D display button and choose real data and contour plot.

The above procedure is automated in an NMRScript, "2D TPPI Processing". To use the script, first process the1D spectrum, then click "Scrits|Processing scripts|2D TPPI Processing".

4. References

1. Derome, A. E, "Modern NMR Techniques for Chemistry Research", Pergamon Press, New York, 1987, p.197 - 227.
2. S. Braun, H.-O. Kalinowski, S. Berger, "150 and More Basic NMR Experiments" Wiley-VCH, Weinheim 1998, p.359 - 361.